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Comparative Evaluation of GC/MS (Gas Chromatography/Mass Spectrometry) Data Analysis Processing

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A COMPARATIVE EVALUATION OF GC/MS DATA ANALYSIS PROCESSING

by

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Using synthetic mixtures the interpretative methods evaluated for accuracy were: (1) manual (skilled interpretor); (2) Incos data software; (3) Mass Spectra Fourier Transformed Search software, and (4) an RTI Mass Spectral Search System. A Rindfleisch deconvolution program was also applied to raw data prior to using the automated procedures. Only manual, Incos, and the RTI system were evaluated with environmental samples. The deconvolution program was also part of this evaluation.

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SECTION 1

INTRODUCTION

The problem of monitoring the environment for the presence of potentially hazardous agents and assessing their capabilities to cause health and ecological effects is enormous. In the United States alone 30,000 to 50,000 chemical substances are produced each year. There are now well over 4 million chemical substances registered with the American Chemical Society Abstract Service and approximately 1,000 new chemicals are developed by industry and placed in commercial usage annually (1). In terms of volume, the production of organic chemicals in the non-Communist world increased from 7 million tons in 1962 to 63 million tons in 1970 and is predicted to increase to 250 million tons by 1985 (2). Further aggravation of this situation is apparent with increasing industrialization in other countries and with increasing world population.

Many of the more dangerous chemical agents have been brought to our attention through occupational exposure incidence and through exposures in the home. For the most part occupational and domestic exposures to hazardous agents have been recognized and dealt with on an individual agent basis. This also has been the case with several incidences of environmental contamination, e.g. the pollution of the James River and surrounding areas by the pesticide Kepone. Clearly, however, the global problem of environmental pollution cannot be approached effectively on a chemical-by-chemical incident-by-incident basis. This is particularly aggravated by the multiplicity of chemicals present at hazardous waste sites.

The fact is that most exposures to hazardous agents in the environment are multi-faceted exposures. Pervasive environmental exposure to multiple agents may pose as yet unrecognized health and ecological risks. If we consider potential long-term health hazards such as cancer with a latency of about 20-30 years, the result of our environmental pollution may not be fully apparent (3).

The high cost and lengthy period for analytical development have precluded the availability of methods which are considered monopollutant methods of analysis. Techniques have been developed which provide a polypollutant analysis of the vapor-phase organics in the atmosphere. However, one of the problems associated with the latter approach is the production of large quantities of data which require computerized techniques to assist in the identification of chemicals in the air samples. The polypollutant method employs gas chromatography/mass spectrometry/computer analysis which may provide both qualitative and quantitative information.

More efficient interpretation of GC/MS/DS data is achieved through the use of computer algorithms spectral searching systems. However computerized systems have not been compared to the manual methods of interpretation and thus, their accuracy is not well documented. Thus, a comparative evaluation of GC/MS data processing techniques was sorely needed.

This research program has addressed the evaluation of three different computer algorithms for spectral identification of chemicals. In addition, an evaluation has been conducted on the ability of the Rindfleisch algorithm (4) to present raw data in a cleaned-up fashion for presentation to the spectral search systems to improve the accuracy of identification. To examine these search algorithms with and without the deconvolution system, the investigation followed a two-pronged approach. First, a series of synthetic mixtures of known composition were prepared which presented the following challenges to the identification routines: (1) overlapping structural characteristics, i.e. similar mass spectra; (2) analyte concentration effects, and (3) compound class effects. A series of chemicals were selected based upon their hazardous nature and of interest to the U.S. Environmental Protection Agency because of their occurrence in environmental ambient air. The second approach was to collect a set of environmental ambient air samples representing diverse atmospheric pollution which could be sampled to challenge the search algorithms. The comparative yardstick was the results from manual interpretation in this case.

Intracomparative evaluations between the three computer algorithms with and without the deconvolution system and manual interpretation are presented in this report.

SECTION 2

CONCLUSIONS

SYNTHETIC MIXTURES

Mass spectra obtained by fused silica capillary GC/MS/DS analysis of mixtures of organic chemicals on Tenax GC® cartridges was subjected to manual and automated interpretative techniques. A total of 85 chemicals representing 15 chemical classes were prepared as various mixtures to simulate the following design effects: (1) the occurrence of similar or dissimilar overlapping mass spectra from two or more constituents present in unresolved gas chromatographic peaks, (2) the occurrence of similar and dissimilar proportions (concentrations) of unresolved components in gas chromatographic peaks, and (3) the use of and presence of different chemical classes in a mixture. Interpretative methods evaluated for accuracy were: (1) manual, (2) Incos data software (Finnigan Corp., San Jose, CA), (3) Mass Spectra Fourier transformed Search (MSFS) analysis, and (4) an RTI Mass Spectral Search System (RTI/MSSS). Furthermore, the Rindfleisch deconvolution (+D) program was also applied to raw data (-D) prior to using the automated procedures.

An evaluation of the effect of similar vs dissimilar mass spectra occurring in an unresolved chromatographic peak revealed that a higher accuracy of identification occurred when the mass spectra was dissimilar. Deconvolution applied to raw data did not appear to improve the accuracy of identification for the automated procedures, whether the spectra were similar or not.

As the level of chemical was increased (50 ng to 5,000 ng/cartridge), the accuracy of identification also increased until the mass spectra became saturated, then the accuracy decreased. The saturation effects (>1,000 ng/cartridge) were observed to decrease accuracy of identification for n-dodecane, n-propyl acetate, di-n-butyl ether, 2-methylbenzofuran, pyridine, m-ethyltoluene, 1,3,5-trimethylbenzene, naphthalene, 2-methylthiophene and acetic acid.

A comparison was made of the ability of each interpretative procedure to accurately identify the chemicals in each mixture. The overall best percent correct identification was achieved with nondeconvoluted (-D) data using the Incos software (75.2%). The remaining procedures ranked as follows: manual (70.7%) > RTI/MSSS (with D, 60.9%) > Incos (with D, 58.2%) > RTI/MSSS (without D, 59.0%) > MSFS (without D, 49.5%) > MSFS (with D, 48.4%). In general, the deconvolution algorithm used did not appear to always aid in correctly identifying chemicals in these synthetic mixtures.

By chemical class, the Incos software performed better on 11 of the 15 classes than other routines, in fact, only manual performed best on the remaining four. Thus, in no cases were the RTI/MSSS or MSFS better for any chemical class than Incos or manual approaches. The following accuracy trends were evident for Incos for the 11 classes: halogenated alkanes (-D, 96.1%) > aromatic aldehydes (-D, 86.7%) > esters (+D, 83.5%) > halogenated aromatics (-D, 83.3%) > ethers (-D, 82.2%) > alkanes (-D, 75.9%) > alcohols (+D, 82.2%) > nitriles (-D, 52.9%) > nitrogen compounds (-D, 47.8%) > acids (-D, 46.7%) > aldehydes (+D, 32.4%). For manual they were: sulfur compounds (95.0%) > aromatics (86.5%) > ketones (81.0%) > phenols (74.4%). The worst results were obtained on alkanes using MSFS (+D, 5.7%).

The automated interpretative methods were compared to manual as to the percentage of the identities that both correctly identified the chemicals in a mixture. The highest percent agreement (-D, 63.6%) was between Incos and manual, while the lowest was manual vs MSFS (+D, 43.0%). When comparing only automated procedures the best agreement (55.3%) was between Incos (-D) and RTI/MSSS (+D).

ENVIRONMENTAL AIR SAMPLES

Because environmental air samples represented truly unknown mixtures, the correct answers were unknown and thus, all comparative statistics on the answers (identities) were made relative to manual interpretation. The following observations were apparent:

(1) a higher percent agreement occurred between manual and RTI/MSSS or Incos methods with the higher volume (thus, higher chemical levels) sampled than with low volume samples;

(2) the application of deconvolution to the raw mass spectra caused the percent agreement to decrease for many samples;

(3) the highest overall agreement (53.9%) across all samples was between manual and Incos (+D);

(4) Incos more often agreed with the answers obtained manually than with the RTI/MSSS when comparing by chemical classes;

(5) aldehydes and halogenated aromatics were always ranked in the top six best agreements regardless of automated method used,

and (6) sulfur compounds always ranked amongst the worst three in percent agreements regardless of the automated method.

SECTION 3

RECOMMENDATIONS

For the chemical classes studied this program established that accuracy can best be achieved by applying either the Incos or manual interpretative procedures. The accuracy is still unacceptably low. Several recommendations are offered:

(1) evaluate additional algorithms, e.g. the STIRRS (Cornell U.);

(2) include the use of relative retention data for chemicals analyzed under the same GC/MS conditions as environmental samples and evaluate the change in accuracy, if any, by their inclusion;

(3) expand the list of chemical classes to include polynuclear aromatics, pesticides, etc.:

(4) attempt to optimize the Reindfleisch deconvolution algorithm;

and (5) after accomplishing items 1-4, above, consider the need for further research on development of automated algorithms, or optimizing those appearing to be most promising.

SECTION 4

EVALUATION OF ALGORITHMS USING SYNTHETIC AIR-VAPOR MIXTURES

INTRODUCTION

The primary objective of these laboratory experiments were to synthesize chemical mixtures of known composition which would adequately test the accuracy of mass spectral software identification systems that have been developed by commercial sources and at universities. A specific aim of this research program was to determine the effects, if any, of overlapping spectra, concentration and compound classes on the accuracy of the identification by software algorithms for various components in a mixture. By testing algorithms with known authentic chemical compositions, the accuracy of identification routines could be assessed. Thus, the first step in their evaluation was to use synthetic mixtures and subsequently, with ambient air samples (Section 5).

Three mass spectral identification search routines were tested with raw mass spectral data and with the same mass spectral data which had been processed through a deconvolution program. The deconvolution program was that of Rindfleisch (4) which was designed to resolve overlapping mass spectra that are present as coeluting compounds in a gas chromatographic peak. The three mass spectral identification search routines that were tested were (a) the INCOS data software supplied on a Data General computer (in this case interfaced to a Finnigan 3300 gas chromatograph/mass spectrometer); (b) a Fourier transform analysis software (MSFS) routine developed by T. Isenhour (5) coupled with a standard EPA mass spectral library, and (c) the Mass Spectral Search Identification Software (RTI/MSSS) routine developed at RTI.

Raw mass spectral data was also interpreted by a skilled investigator who had no knowledge of the composition of the synthetic mixtures.

EXPERIMENTAL PROCEDURES

Chemicals Selected for Evaluation of Algorithms

The chemicals selected for this evaluation are shown in Table 1. A series of compounds represent ; alkanes, alcohols, aldehydes, esters, ethers, ketones, nitriles, nitrogen compounds, aromatics, halogenated alkanes, halogenated aromatics, aromatic aldehydes, sulfur compounds, acids and phenols was selected because many of these chemicals have been identified in ambient air samples which have been collected throughout the Continental U.S. Also their selection was based on their hazardous nature and are of interest to the EPA. These chemicals in many cases are only partially resolved as gas chromatographic peaks, i.e. they occur as overlapping components in the chromatographic peak. Table 2 indicates which chemicals were partially resolved with gas chromatography. (These chemicals were analyzed by gas chromatography with flame ionization detection to establish their retention times.)

This set of chemicals, provided the potential to achieve the three primary aims, i.e., overlapping spectral, concentration, and compound class effects on the accuracy of mass spectral search identification routines.

Chromatographic Conditions

To construct the desired mixtures, preliminary work involved determining the retention times of components. High resolution gas chromatography with flame ionization detection was employed and the parameters used are shown in Table 3. Upon analysis of the compounds they were arranged in order and grouped with respect to retention time and resolution from neighboring peaks, respectively. These results were shown in Table 2.

Using these data, mixtures of appropriate compounds were loaded onto Tenax cartridges to provide samples for gas chromatographic/mass spectrometric (GC/MS) analysis (6). The mixtures were prepared to evaluate the effects described earlier. A total of nineteen Tenax cartridges were loaded with the appropriate compounds to provide these effects. The levels employed (L, M, H, HS, Table 4) and their compositions are given in Tables 5-11. Table 4 provides a general key for the levels of chemicals loaded onto the Tenax cartridges.

Analysis of Synthetic Mixtures By GC/MS

The nineteen Tenax GC cartridges presented in the previous tables were analyzed by capillary GC/MS with an INCOS data acquisition system. The mass

Table 1. CHEMICALS USED IN EVALUATIONS

Chemical Class:	Alkanes 1	Alcohols 2	Aldehydes 3	Esters 4	Ethers 5
	n-Hexane	Methanol	Acrolein	Ethyl acetate	Diethyl ether
	n-Heptane	Ethanol	Propionaldehyde	Methyl methacrylate	2-Methyl furan
	n-Octane	t-Butanol	Heptaldehyde	Ethyl acrylate	Di-n-butyl ether
	n-Decane		n-Undecanal	n-Propyl acetate	Methylbenzofuran
	n-Undecane			n-Butyl acetate	
	n-Dodecane			Butyl acrylate	
	n-Tridecane			n-Butyl methacrylate	

(continued)

Table 1 (cont'd.)

Chemical Class:	Ketones 6	Nitriles 7	Nitrogen Compounds 8	Aromatics 9
	Methyl vinyl ketone	Acetonitrile	Pyridine	Benzene
	2-Petanone	Acrylonitrile	Nitrobenzene	Toluene
	3-Pentanone	α-Methylbutyronitrile	Piperidine	o-Xylene
	Cyclohexanone	Benzonitrile	Pyrrolidine	m-Xylene
	Acetophenone		Quinoline	m-Ethyltoluene
	Propiophenone			p-Ethyltoluene
	Acetone			1,2,3-Trimethylbenzene
				1,3,5-Trimethylbenzene
				Naphthalene
				Ethylbenzene
				Styrene

(continued)

Table 1 (cont'd.)

Chemical Class:	Halogenated Alkenes 10	Halogenated Aromatics 11	Aromatic Aldehydes 12
	Vinyl chloride	Chlorobenzene	Benzaldehyde
	Methyl bromide	m-Dichlorobenzene	Tolualdehyde
	Vinylidene chloride	p-Dichlorobenzene	Dichlorobenzaldehyde
	Methylene chloride	Trichlorobenzene	
	1,1-Dichloroethane	Perfluorobenzene	
	1,1,1-Trichloroethane	Perfluorotoluene	
	1,2-Dichloroethane	o-Chloronitrobenzene	
	1,2-Dichloropropane		
	Trichloroethylene		
	Tetrachloroethylene		
	Chloroform		
	1,1,2,2-Tetrachloroethane		
	Hexachloro-1,3-butadiene		

(continued)

Table 1 (cont'd.)

Chemical Class:	Sulfur Compounds 13	Acids 14	Phenols 15
	Thiophene	Acetic	m-Cresol
	Methylthiophene	n-Butyric	o-Cresol
	Benzothiophene		p-Cresol
	Benzothiazole		Phenol

Table 2. COMPOUNDS LOADED INTO TENAX CARTRIDGE 20 - ENTIRE SET OF CHEMICALS

Approximate Retention Time (min)	Compound	Level of Compound Loaded Cartridge #20
4.07	methanol	M
4.08	methyl bromide	H
4.37	vinyl bromide	H
4.52	acrolein	M
4.56	acetonitrile	M
4.59	propionaldehyde	M
4.60	acetone	M
4.84	diethyl ether	M
4.88	ethanol	M
4.97	acrylonitrile	M
4.98	vinylidene chloride	M
5.10	methylene chloride	M
5.27	t-butanol	M
5.94	nitromethane	M
5.90	1,1-dichloroethane	H
6.28	methyl vinyl ketone	M
6.62	2-methylfuran	M
6.62	perfluorobenzene	M
6.69	n-hexane	M
6.80	ethyl acetate	M
6.84	chloroform	M
7.46	perfluorotoluene	M
7.60	1,2-dichloroethane	H
7.79	1,1,1-trichloroethane	M
8.34	benzene	H
8.53	thiophene	M
9.09 (tent.)	pyrrolidine	M
9.10	2-pentanone	M
-[a]	acetic acid	M
~9.30	1,2-dichloropropane	M
9.36	3-pentanone	M
9.44	ethyl acrylate	M
9.70	trichloroethylene	H

(continued)

Table 2 (cont'd.)

Approximate Retention Time (min)	Compound	Level of Compound Loaded Cartridge #20
10.08	methyl methacrylate	M
10.09	n-heptane	M
10.23	n-propyl acetate	M
10.34	α-methylbutyronitrile	M
11.41 (tent.)	piperidine	M
11.46	pyridine	M
12.74	toluene	M
12.90	2-methylthiophene	M
14.86	butyl acetate	M
14.90	n-octane	M
15.08	tetrachloroethylene	M
16.77	chlorobenzene	M
17.77	ethylbenzene	L
18.24	m-xylene	M
18.34	p-xylene	M
18.74	cyclohexanone	M
19.19	di-n-butyl ether	M
19.32	n-butyl acrylate	M
19.32	styrene	M
19.50	heptaldehyde	M
19.58	o-xylene	M
19.70	1,1,2,2-tetrachloroethane	M
20.62	anisole	M
22.74	benzaldehyde	M
23.61	m-ethyltoluene	M
23.63	benzonitrile	M
23.77	p-ethyltoluene	M
24.12	1,3,5-trimethylbenzene	M
24.28	butyl methacrylate	M
24.30	phenol	M
25.95	m-dichlorobenzene	M

(continued)

Table 2 (cont'd.)

Approximate Retention Time (min)	Compound	Level of Compound Loaded Cartridge #20
26.32	p-dichlorobenzene	M
26.34	n-decane	M
27.28	1,2,3-trimethylbenzene	H
28.44	o-cresol	M
28.89	acetophenone	M
29.58	p-cresol	M
29.66	m-cresol	M
29.82	nitrobenzene	M
29.88	p-tolualdehyde	M
31.84	2-methylbenzofuran	M
32.02	n-undecane	M
32.39	n-ethylaniline	M
34.44	propiophenone	M
34.85	ethyl benzoate	M
35.81	1,2,4-trichlorobenzene	M
36.11	naphthalene	M
36.42	1-benzothiophenone	M
37.46	n-dodecane	M
37.80	2-benzothiazole	M
38.23	hexachloro-1,3-butadiene	M
38.33	o-chloronitrobenzene	M
38.64	quinoline	M
39.19	n-butyrophenone	M
40.98	3,4-dichlorobenzaldehyde	M
41.78	n-undecanal	M
42.48	n-tridecane	M
43.2 (est.)	n-butyric acid	M

[a]Elution expected at this point according to other data. No elution was observed during screening of the compounds.

Table 3. HRGC/FID OPERATING CONDITIONS FOR QUALITATIVE ANALYSTS OF THE TEST COMPOUNDS

Parameter	Description/Setpoint
Column	25 m bonded methyl silicone fused silica capillary
Inner diameter	0.32 mm
Film thickness	1.0 μ
He Carrier Flow	1.23 mL/min
He make-up flow	15.9 mL/min
Temperature program	35°C (0 min) → 175°C @ 3°C/min
Injection temperature	280°C
Detector temperature	300°C
Detector	Flame ionization
H_2 flow	47 mL/min
Air flow	280 mL/min
Desorption unit	
Block temperature	260°C
Trap temperatures	-196°C to +250°C
He flow	12.6 mL/min
Desorption time	8.0 min
Transfer line temperature	220°C

Table 4. KEY TO LEVELS OF COMPOUNDS LOADED INTO TENAX CARTRIDGES FOR QUALITATIVE ANALYSIS

Level	Symbol	Mass Range (Ng/Cartridge)
Low	L	50-200
Moderate	M	201-650
High	H	651-1500
Very high (saturated)	HS	1501-5000

Table 5. MIXTURES WITH UNRESOLVED DOUBLETS LOADED ONTO TENAX CARTRIDGES 1, 2, and 3 - SIMILAR MASS SPECTRA

Compound	Level of Compound Loaded		
	Cart. #1	Cart. #2	Cart. #3
Acrolein	M	H	L
Acetonitrile	M	L	H
2-Methylfuran	M	H	L
Ethyl acetate	M	L	H
Pyrrolidine	M	H	L
2-Pentanone	M	L	H
3-Pentanone	M	H	L
Ethyl acrylate	M	L	H
n-Propyl acetate	M	H	L
α-Methylbutyronitrile	M	L	H
m-Xylene	M	H	L
p-Xylene	M	L	H
Di-n-butyl ether	M	H	L
n-Butyl acrylate	M	L	H
m-Ethyltoluene	M	H	L
p-Ethyltoluene	M	L	H
p-Cresol	M	H	L
m-Cresol	M	L	H

Table 6. MIXTURES WITH UNRESOLVED DOUBLETS LOADED ONTO TENAX CARTRIDGES 4, 5, AND 6 - DISSIMILAR MASS SPECTRA

Compound	Level of Compound Loaded		
	Cart. #4	Cart. #5	Cart. #6
Propionaldehyde	M	H	L
Acetone	M	L	H
Methylene chloride	M	H	L
t-Butanol	M	L	H
2-Methylfuran	M	L	H
Perfluorobenzene	M	H	L
Perfluorotoluene	M	H	L
1,2-Dichloroethane	H	L	H
Benzene	H	L	H
Thiophene	M	H	L
2-Pentanone	M	H	L
Acetic acid	M	L	H
Methyl methacrylate	M	H	L
n-Heptane	M	L	H
Piperidine	M	H	L
Pyridine	M	L	M
Toluene	M	L	H
2-Methylthiophene	M	H	L
Butyl acetate	M	H	L
n-Octane	M	L	M
Styrene	M	H	L
Heptaldehyde	M	L	H
m-Ethyltoluene	M	H	L
Benzonitrile	M	L	H
1,3,5-Trimethylbenzene	M	H	L
Butyl methacrylate	M	L	H
p-Dichlorobenzene	M	H	L
n-Decane	M	L	H
Nitrobenzene	M	L	H
p-Tolualdehyde	M	H	L

(continued)

Table 6 (cont'd.)

Compound	Level of Compound Loaded		
	Cart. #4	Cart. #5	Cart. #6
2-Methylbenzofuran	M	H	L
n-Undecane	M	L	H
Naphthalene	M	H	L
1-Benzothiophene	M	L	H
n-Dodecane	M	H	L
2-Benzothiazole	M	L	H
Hexachloro-1,3-butadiene	M	L	H
o-Chloronitrobenzene	M	H	L

Table 7. MIXTURES WITH UNRESOLVED TRIPLETS LOADED INTO TENAX CARTRIDGES 7, 8, and 9

Compound	Level of Compound Loaded		
	Cart. #7	Cart. #8	Cart. #9
Acetonitrile	M	L	H
Propionaldehyde	M	H	L
Acetone	M	L	L
Vinylidene chloride	M	L	H
Methylene chloride	M	H	L
t-Butanol	M	L	L
2-Methylfuran	M	L	L
Perfluorobenzene	M	H	L
n-Hexane	M	L	H
Perfluorotoluene	M	H	L
1,2-Dichloroethane	H	L	L
1,1,1-Trichloroethane	M	L	H
Benzene	H	L	H
Thiophene	M	H	L
2-Pentanone	M	H	L
Acetic acid	M	L	L
1,2-Dichloropropane	M	L	H
Methyl methacrylate	M	H	L
n-Heptane	M	L	L
n-Propyl acetate	M	L	H
Piperidine	M	H	L
Pyridine	M	L	H
Toluene	M	L	H
2-Methylthiophene	M	H	L
Butyl acetate	M	H	L
n-Octane	M	L	L
Tetrachloroethylene	M	L	H
Styrene	M	H	L
Heptaldehyde	M	L	L
o-Xylene	M	L	H
m-Ethyltoluene	M	H	L
Benzonitrile	M	L	L
p-Ethyltoluene	M	L	H

(continued)

Table 7 (cont'd.)

Compound	Level of Compound Loaded		
	Cart. #7	Cart. #8	Cart. #9
1,3,5-Trimethylbenzene	M	H	L
Butyl methacrylate	M	L	L
Phenol	M	L	H
p-Dichlorobenzene	M	H	L
n-Decane	M	L	H
m-Cresol	M	L	H
Nitrobenzene	M	L	L
p-Tolualdehyde	M	H	L
2-Methylbenzofuran	M	H	L
n-Undecane	M	L	H
Naphthalene	M	H	L
1-Benzothiophene	M	L	H
n-Dodecane	M	H	L
2-Benzothiazole	M	L	H
Heptachloro-1,3-butadiene	M	L	L
o-Chloronitrobenzene	M	H	L
Quinoline	M	L	H

Table 8. MIXTURES WITH UNRESOLVED QUARTETS LOADED INTO CARTRIDGES 10, 11, AND 12

Compound	Level of Compound Loaded		
	Cart. #10	Cart. #11	Cart. #12
Acrolein	M	H	L
Acetonitrile	M	L	L
Propionaldehyde	M	L	HS
Acetone	M	L	L
Acrylonitrile	M	H	L
Vinylidene chloride	M	L	L
Methylene chloride	M	L	HS
t-Butanol	M	L	L
2-Methylfuran	M	L	L
Perfluorobenzene	M	L	HS
n-Hexane	M	L	L
Ethyl acetate	M	H	L
Perfluorotoluene	M	L	HS
1,2-Dichloroethane	H	L	L
1,1,1-Trichloroethane	M	L	L
Benzene	H	L	L
Thiophene	M	L	HS
Pyrrolidine	M	H	L
2-Pentanone	M	L	HS
Acetic acid	M	L	L
1,2-Dichloropropane	M	L	L
Methyl methacrylate	M	L	HS
n-Heptane	M	L	L
n-Propyl acetate	M	L	L
α-Methylbutyronitrile	M	H	L
Piperidine	M	L	HS
Pyridine	M	L	L
Toluene	M	L	L
2-Methylthiophene	M	L	HS
Butyl acetate	M	L	HS
n-Octane	M	L	L
Tetrachloroethylene	M	L	L

(continued)

Table 8 (cont'd.)

Compound	Level of Compound Loaded		
	Cart. #10	Cart. #11	Cart. #12
n-Butyl acrylate	M	H	L
Styrene	M	L	HS
Heptaldehyde	M	L	L
o-Xylene	M	L	L
m-Ethyltoluene	M	L	HS
Benzonitrile	M	L	L
p-Ethyltoluene	M	L	L
1,3,5-Trimethylbenzene	M	L	HS
Butyl methacrylate	M	L	L
Phenol	M	L	L
p-Dichlorobenzene	M	L	HS
n-Decane	M	L	L
p-Cresol	M	H	L
m-Cresol	M	L	L
Nitrobenzene	M	L	L
p-Tolualdehyde	M	L	HS
2-Methylbenzofuran	M	L	HS
n-Undecane	M	L	L
Naphthalene	M	L	HS
1-Benzothiophene	M	L	L
n-Dodecane	M	L	HS
2-Benzothiazole	M	L	L
Hexachloro-1,3-butadiene	M	L	L
o-Chloronitrobenzene	M	L	HS
Quinoline	M	L	L

Table 9. MIXTURES WITH UNRESOLVED QUINTETS LOADED INTO TENAX CARTRIDGES 13, 14, AND 15

Compound	Level of Compound Loaded		
	Cart. #13	Cart. #14	Cart. #15
Acrolein	M	H	L
Acetonitrile	M	L	L
Propionaldehyde	M	L	H
Acetone	M	L	L
Ethanol	M	L	L
Acrylonitrile	M	H	L
Vinylidene chloride	M	L	L
Methylene chloride	M	L	H
t-Butanol	M	L	L
2-Methylfuran	M	L	L
Perfluorobenzene	M	L	H
n-Hexane	M	L	L
Ethyl acetate	M	H	L
Chloroform	M	L	L
Perfluorotoluene	M	L	H
1,2-Dichloroethane	H	L	L
1,1,1-Trichloroethane	M	L	L
Benzene	H	L	L
Thiophene	M	L	H
Pyrrolidine	M	H	L
2-Pentanone	M	L	H
Acetic acid	M	L	L
1,2-Dichloropropane	M	L	L
3-Pentanone	M	L	L
Methyl methacrylate	M	L	H
n-Heptane	M	L	L
n-Propyl acetate	M	L	L
α-Methylbutyronitrile	M	H	L
Piperidine	M	L	H
Pyridine	M	L	L
Toluene	M	L	L
2-Methylthiophene	M	L	H
Butyl acetate	M	L	H
n-Octane	M	L	L
Tetrachloroethylene	M	L	L

(continued)

Table 9 (cont'd.)

Compound	Level of Compound Loaded		
	Cart. #13	Cart. #14	Cart. #15
Di-n-butyl ether	M	L	L
n-Butyl acrylate	M	H	L
Styrene	M	L	H
Heptaldehyde	M	L	L
o-Xylene	M	L	L
m-Ethyltoluene	M	L	H
Benzonitrile	M	L	L
p-Ethyltoluene	M	L	L
1,3,5-Trimethylbenzene	M	L	H
Butyl methacrylate	M	L	L
Phenol	M	L	L
p-Dichlorobenzene	M	L	H
n-Decane	M	L	L
p-Cresol	M	H	L
m-Cresol	M	L	L
Nitrobenzene	M	L	L
p-Tolualdehyde	M	L	H
2-Methylbenzofuran	M	L	H
n-Undecane	M	L	L
Naphthalene	M	L	H
1-Benzothiophene	M	L	L
n-Dodecane	M	L	H
2-Benzothiazole	M	L	L
Hexachloro-1,3-butadiene	M	L	L
o-Chloronitrobenzene	M	L	H
Quinoline	M	L	L

Table 10. MIXTURES WITH UNRESOLVED SEXTETS LOADED INTO TENAX CARTRIDGES 16, 17, AND 18

Compound	Level of Compound Loaded		
	Cart. #16	Cart. #17	Cart. #18
Acrolein	M	L	L
Acetonitrile	M	L	H
Propionaldehyde	M	H	L
Acetone	M	L	L
Diethyl ether	M	L	L
Ethanol	M	L	L
Acrylonitrile	M	L	L
Vinylidene chloride	M	L	H
Methylene chloride	M	H	L
t-Butanol	M	L	L
2-Methylfuran	M	L	L
Perfluorobenzene	M	H	L
n-Hexane	M	L	H
Ethyl acetate	M	L	L
Chloroform	M	L	L
Perfluorotoluene	M	H	L
1,2-Dichloroethane	H	L	L
1,1,1-Trichloroethane	M	L	H
Benzene	H	L	L
Thiophene	M	H	L
Pyrrolidine	M	L	L
2-Pentanone	M	H	L
Acetic acid	M	L	L
1,2-Dichloropropane	M	L	H
3-Pentanone	M	L	L
Ethyl acrylate	M	L	L
Methyl methacrylate	M	H	L
n-Heptane	M	L	L
n-Propyl acetate	M	L	H
α-Methylbutyronitrile	M	L	L
Piperidine	M	H	L
Pyridine	M	L	L
Toluene	M	L	L
2-Methylthiophene	M	H	L
Butyl acetate	M	H	L
n-Octane	M	L	L
Tetrachloroethylene	M	L	H

(continued)

Table 10 (cont'd.)

Compound	Level of Compound Loaded		
	Cart. #16	Cart. #17	Cart. #18
Di-n-butyl ether	M	L	L
n-Butyl acrylate	M	L	L
Styrene	M	H	L
Heptaldehyde	M	L	L
o-Xylene	M	L	H
1,1,2,2-Tetrachloroethane	M	L	L
m-Ethyltoluene	M	H	L
Benzonitrile	M	L	L
p-Ethyltoluene	M	L	H
1,3,5-Trimethylbenzene	M	H	L
Butyl methacrylate	M	L	L
Phenol	M	L	H
p-Dichlorobenzene	M	H	L
n-Decane	M	L	L
p-Cresol	M	L	L
m-Cresol	M	L	H
Nitrobenzene	M	L	L
p-Tolualdehyde	M	H	L
2-Methylbenzofuran	M	H	L
n-Undecane	M	L	L
Naphthalene	M	H	L
1-Benzothiophene	M	L	L
n-Dodecane	M	H	L
2-Benzothiazole	M	L	L
Hexachloro-1,3-butadiene	M	L	L
o-Chloronitrobenzene	M	H	L
Quinoline	M	L	H

Table 11. HIGHLY VOLATILE MIXTURE LOADED INTO TENAX CARTRIDGE 19

Compound	Level of Compound Loaded
	Cart. #19
Methanol	M
Methyl bromide	H
Vinyl bromide	H

spectrometer was a Finnigan 3300 quadrupole instrument. The operating conditions for thermal desorption and gas chromatography were identical to those described in Table 1 and in fact the same fused silica capillary employed with the GC/FID analysis was used here.

The GC/MS analysis was conducted within 24 h of preparing the synthetic mixtures on the Tenax GC cartridges. The analysis of the 20 cartridges required 2 1/2 days of operating time. Thus, each of the mixtures that was prepared was stored no longer than 48 h prior to analysis to reduce potential variability that might occur. All of the GC/MS data obtained from the MS analysis were acquired onto a hard disk and archived on a magnetic tape. The processing of these data are described below.

Automated and Manual Interpretative Techniques

The identification algorithms employed on the data for identification of chemicals were (1) manual interpretation (composition was unknown to interpretor); (2) the RTI/MSSS; (3) the MSFS, and (4) the INCOS system. The use of the Incos software for identification of chemicals employed the chromatographic peak-top enhancement algorithm, a form of spectral deconvolution. The operator decided the location of the peaktop by inspecting the ion chromatograms and mass spectra in concert with the peak-top enhancement routine. Thus, the operator, not the computer selected the mass spectrum to be submitted to the Incos search algorithm.

Figure 1 is a schematic showing data acquisition and data processing (either as raw data or as data from the Rindfleisch cleanup algorithm) by the search systems. Thus, except for the manual method which compared mass spectra to the Eight Peak Index (7) and Wiley Library (8) and did not employ knowledge of retention times, each of the algorithms were compared with and without the Rindflesich deconvolution system. The mass spectra from the nineteen mixtures shown in Tables 4-10 were submitted to this routine.

RESULTS AND DISCUSSION

Chromatography of Mixtures

As indicated in Tables 4-10 the synthetic mixtures were constructed in order to provide a design effect which included (1) overlapping mass spectra; (2) concentration effects, and (3) increasing complexity. A relatively short

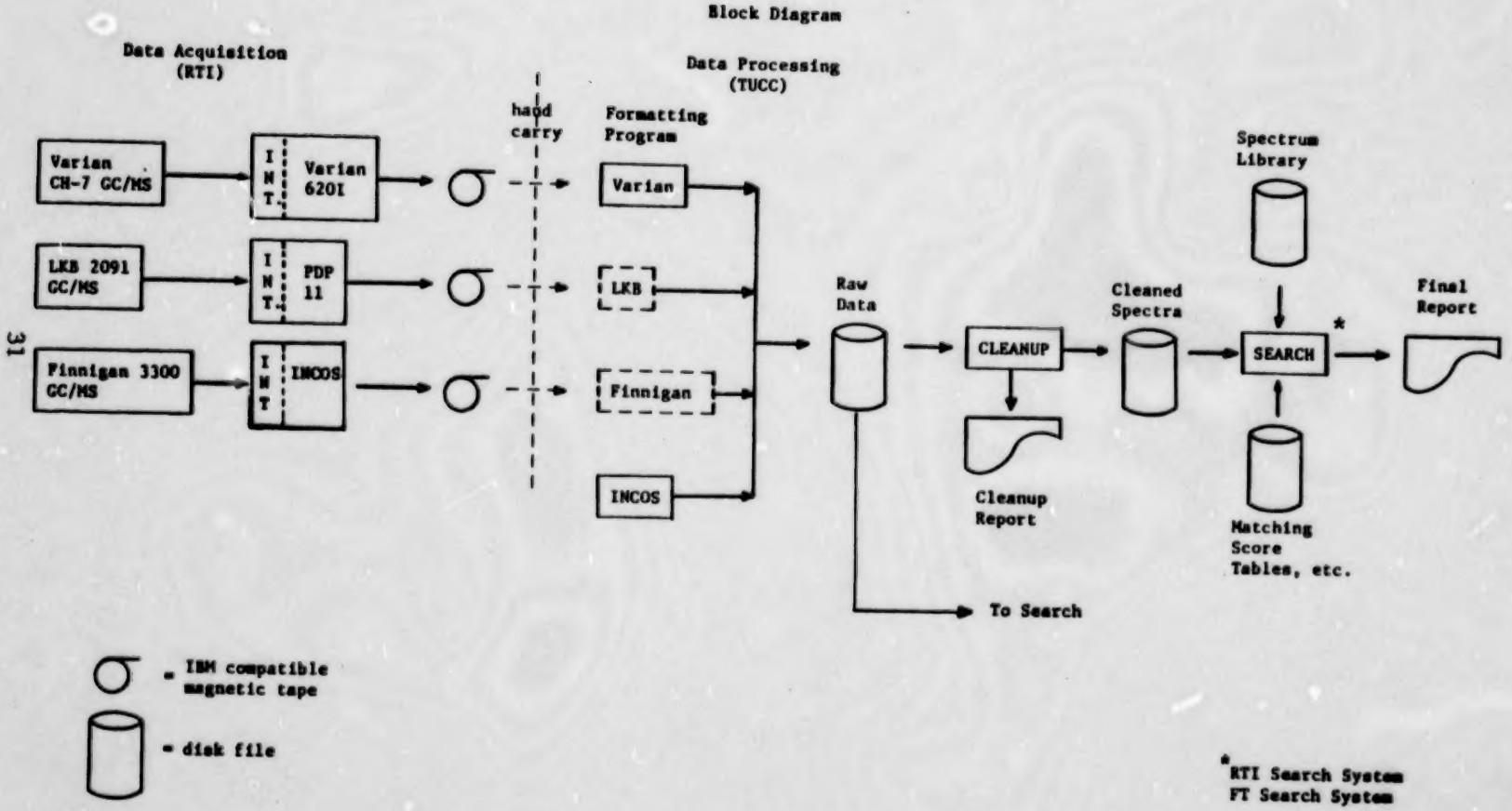

Figure 1. RTI Mass Spectral Identification System (MSSS).

fused silica capillary (30 M DB-1) was used to deliberately produce partially resolved gas chromatographic peaks.

The chromatography of these mixtures are shown in Figures 2-9. A representative chromatogram is depicted from each of the design conditions given in Tables 4-10. The other mixtures that were analyzed by GC/MS varied as to concentration of the components within the convoluted peaks.

For the most part the chromatographic column yielded symmetrical peaks with a minimal amount of tailing, even with some of the more polar substances such as the acids and bases.

Qualitative Analysis

Except for manual interpretation of raw data, the computer algorithms provided a ranking value (for Incos, RFit was used) with each analyte identity in the sample. For each algorithm the five best ranking values were provided to examine those identifications being incorrect as first choices but correctly represented as lower choices. Table 12 presents the ranking definitions used to score the results. A summary of the identity results for each mixture is presented in Appendix A.

The data were assigned the corresponding ranking values as indicated in Table 12 and then the information was sorted to gain insight into the original objectives.

Table 13 presents the overall percent correct identities by the method of identification (includes data from all mixtures). These results clearly indicate that the highest percent accuracy was obtained with manual interpretation and the use of the INCOS algorithm on the Nova Data General computer. Also the accuracy was higher for nondeconvoluted data than after the raw data was subjected to the Rindfleisch deconvolution algorithm. The poorest results were obtained with the Fourier transform mass spectral search algorithm. It achieved only 49% correct identifications. On an overall basis, the application of the Rindfleisch deconvolution algorithm to raw data prior to subjecting the mass spectra to the various identification routines appeared to have very little effect on increasing the percent of the chemicals correctly identified.

In the previous Tables 4-10 the composition of the various mixtures was presented and their corresponding concentrations. These compositions were designed to mimic conditions producing doublets with similar or dissimilar

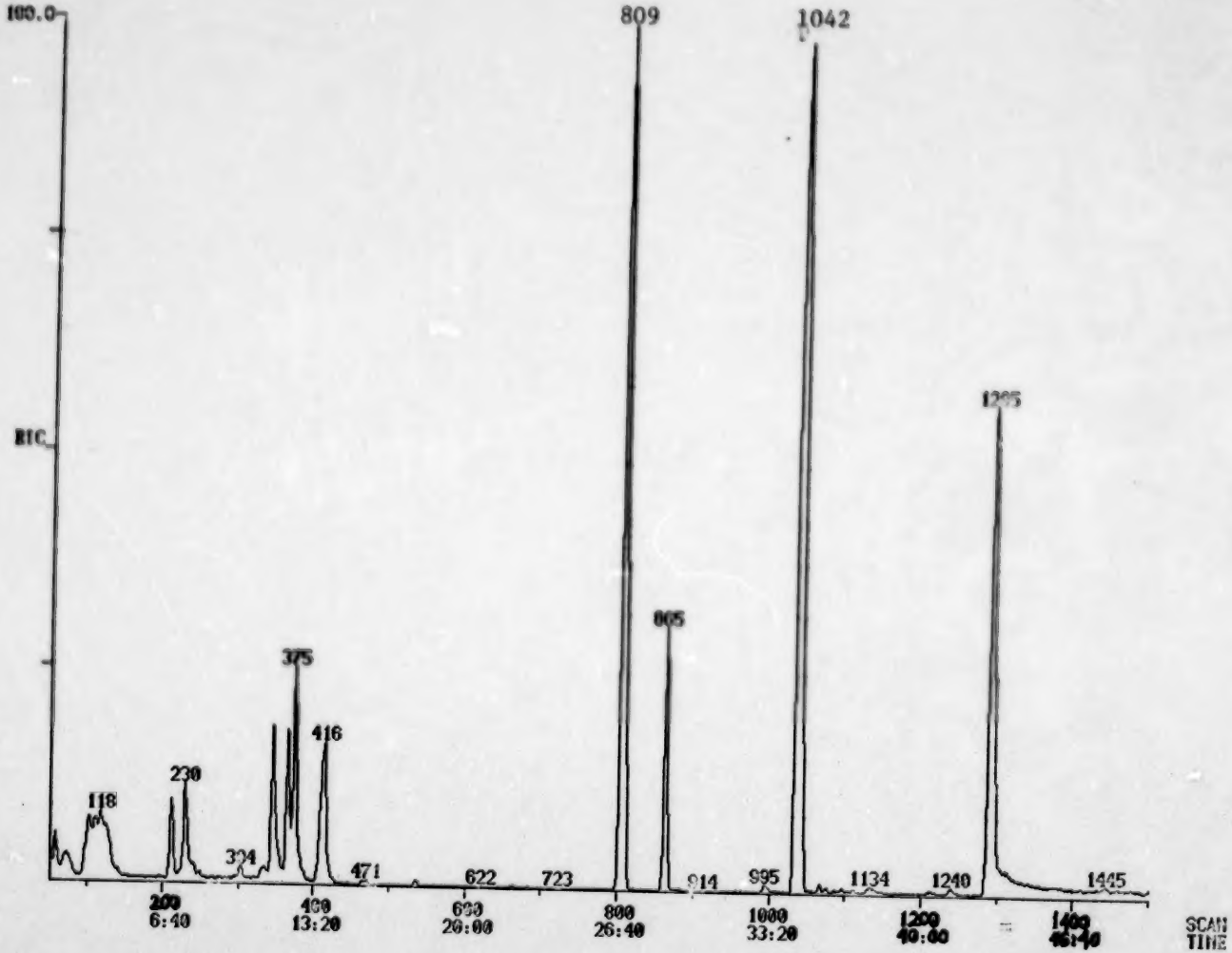

Figure 2. Reconstructed ion chromatogram of mixture with unresolved doublets and similar mass spectra (see Table 4, Cartridge 1).

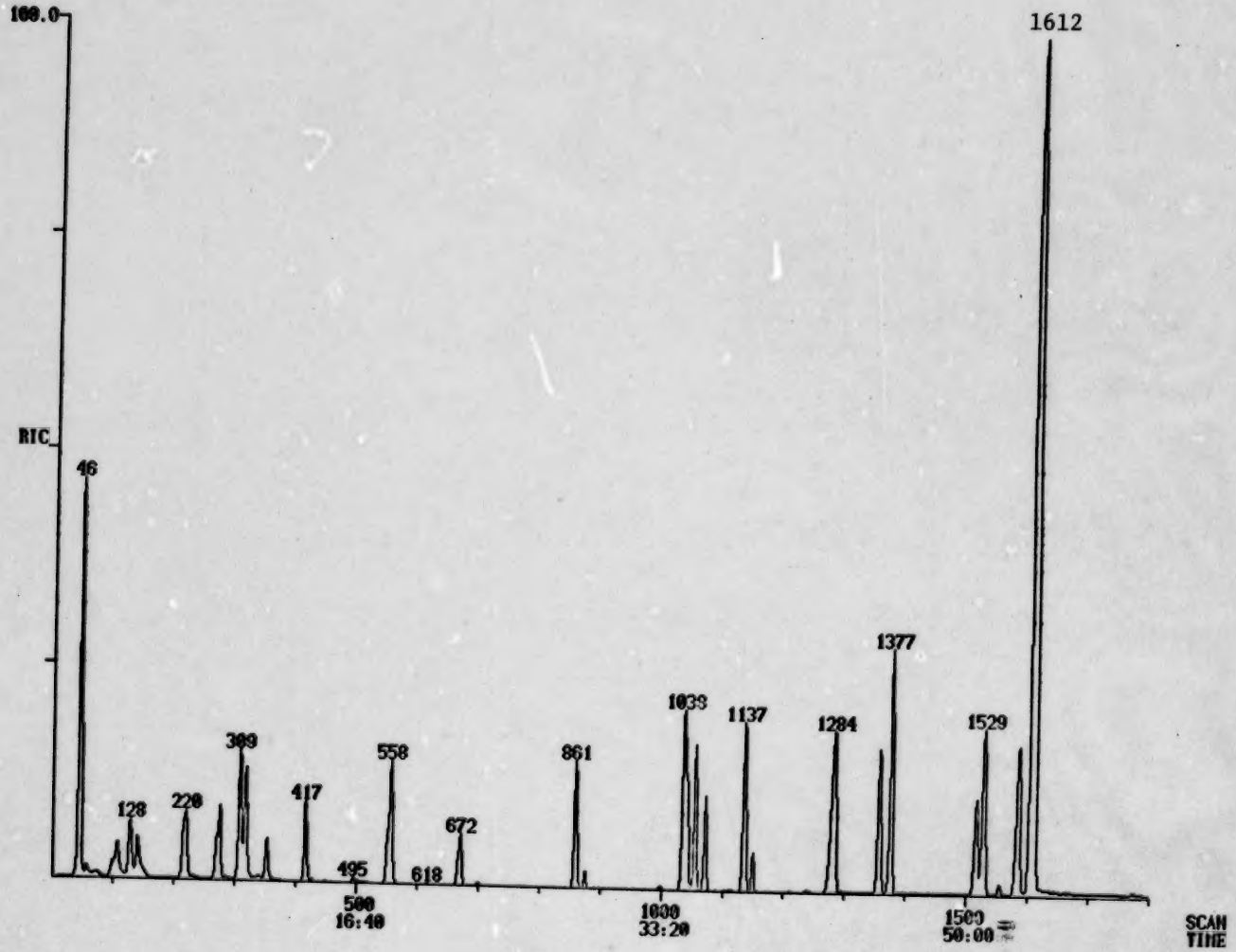

Figure 3. Reconstructed ion chromatogram of mixture with unresolved doublets and dissimilar mass spectra (see Table 5, Cartridge 4).

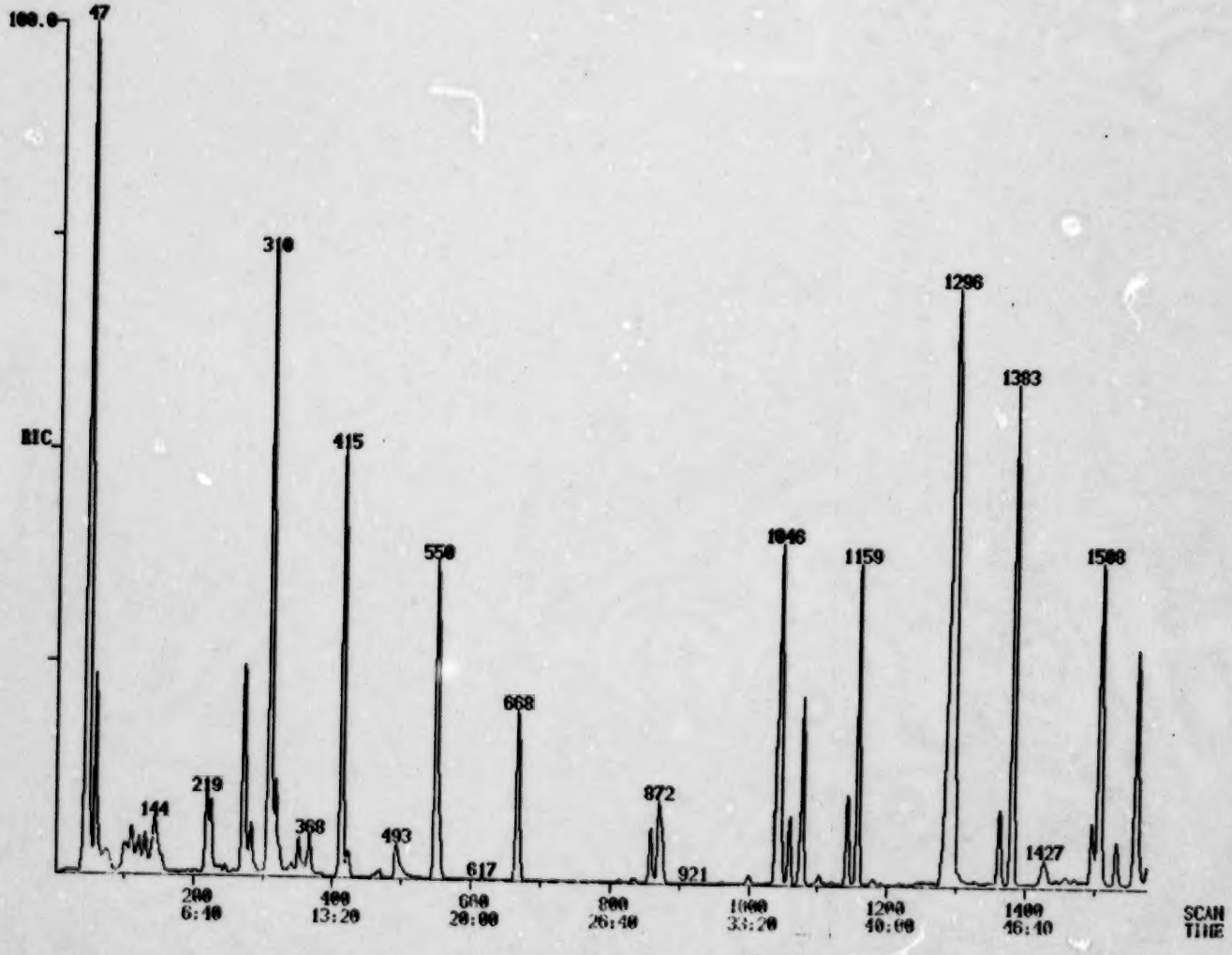

Figure 4. Reconstructed ion chromatogram of mixture with unresolved triplets (see Table 6, Cartridge 8).

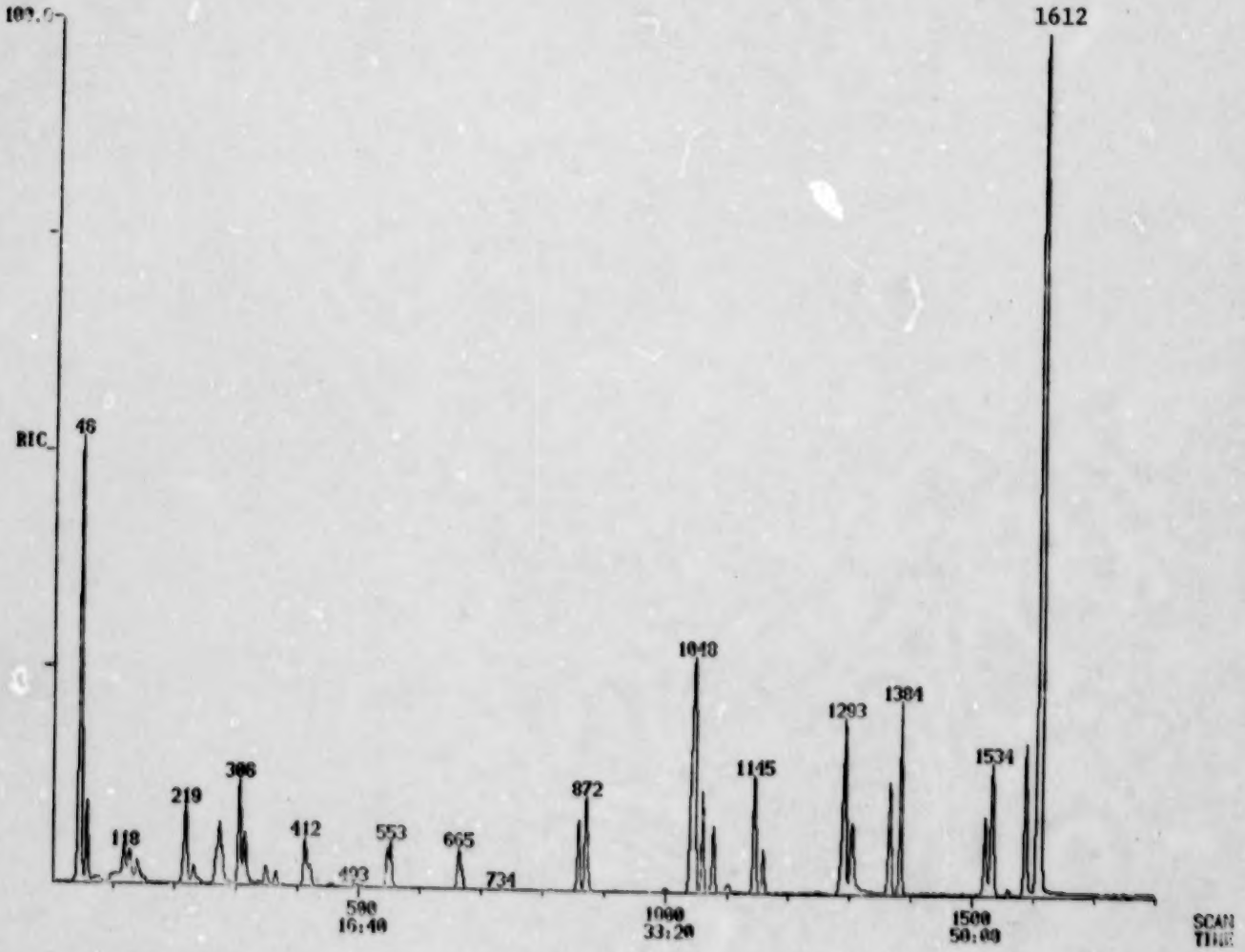

Figure 5. Reconstructed ion chromatogram of mixture with unresolved quartets (see Table 7, Cartridge 10).

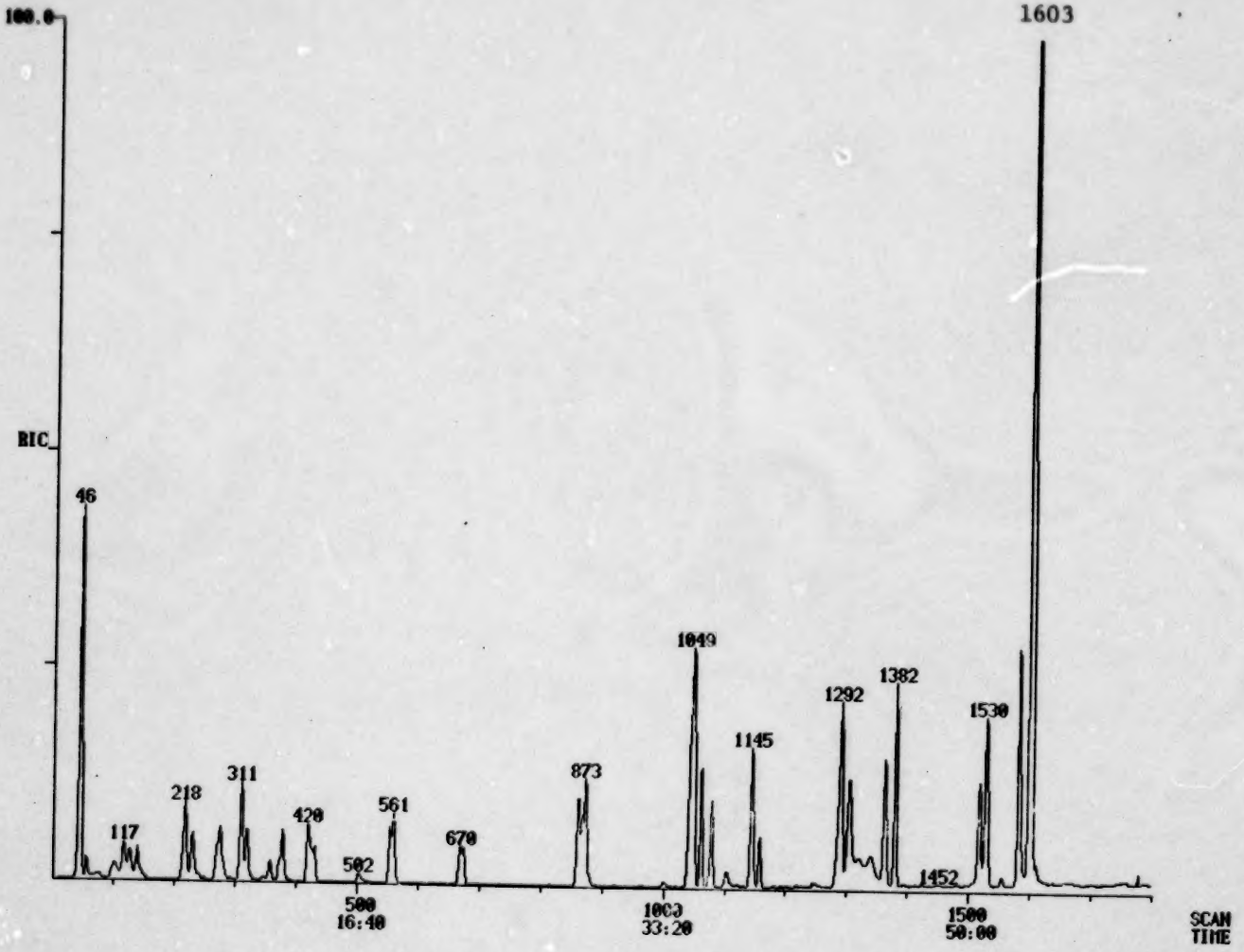

Figure 6. Reconstructed ion chromatogram of mixture with unresolved quintets (see Table 8, Cartridge 13).

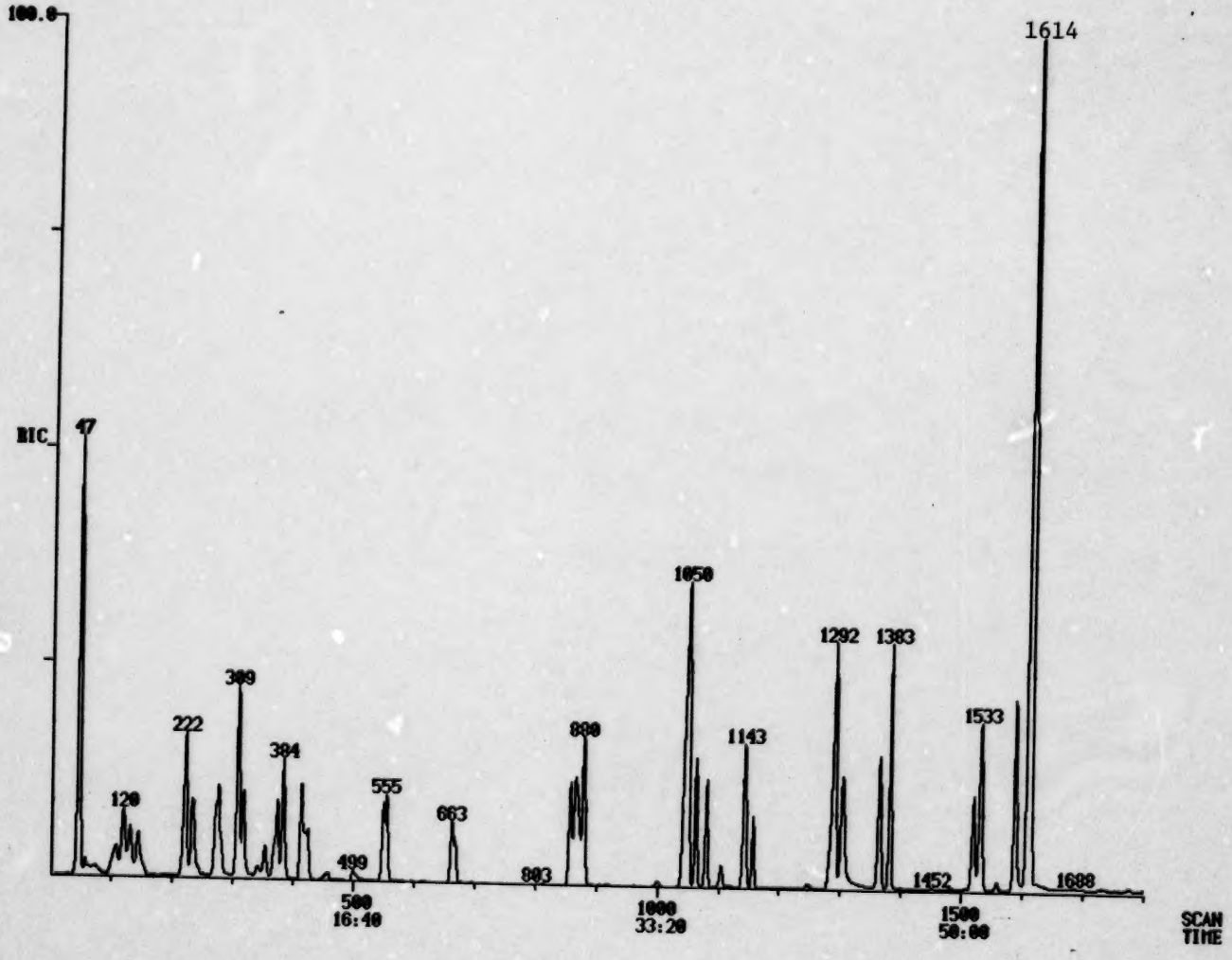

Figure 7. Reconstructed ion chromatogram of mixture with unresolved sextets (see Table 9, Cartridge 16).

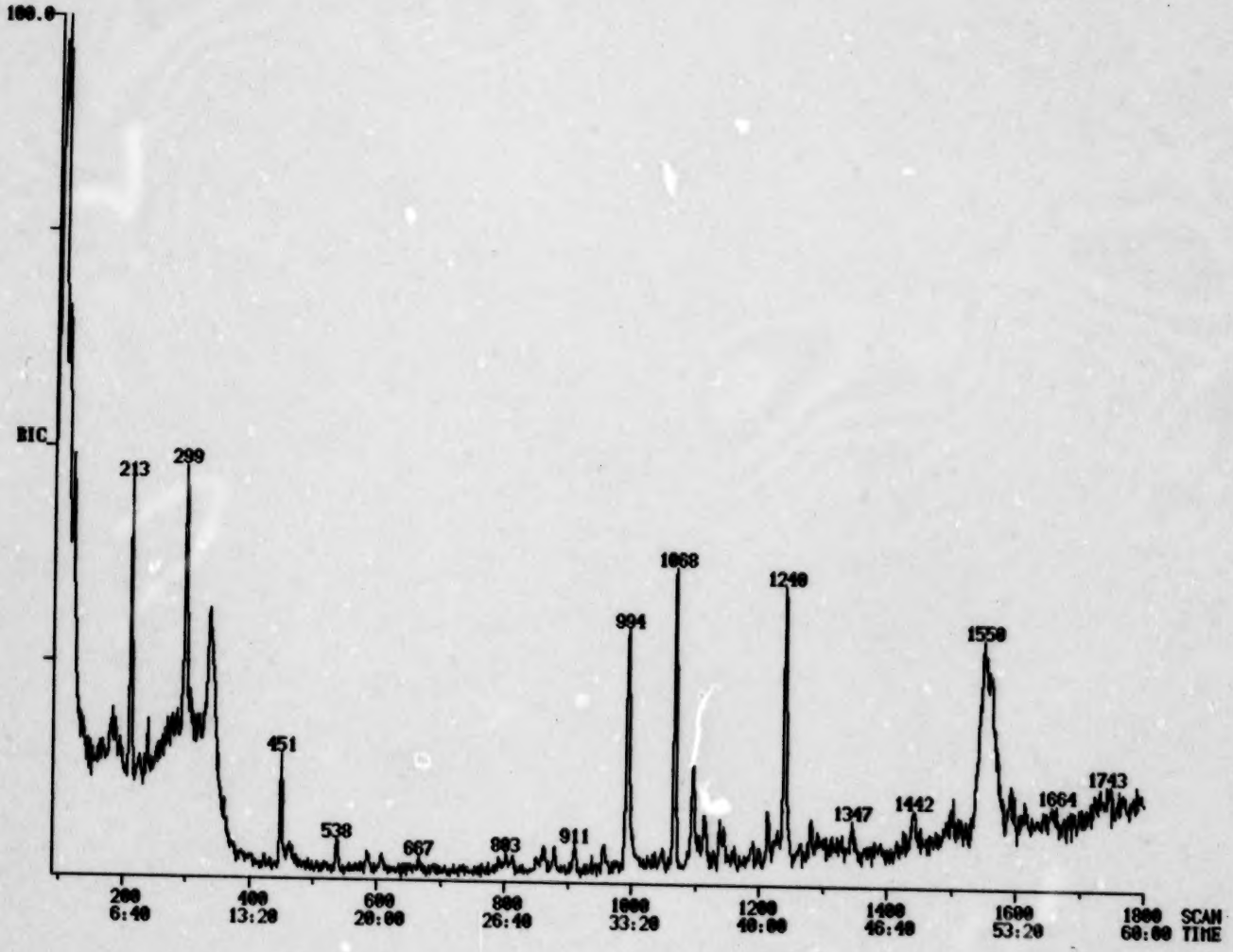

Figure 8. Reconstructed ion chromatogram of highly volatile compounds (see Table 10).

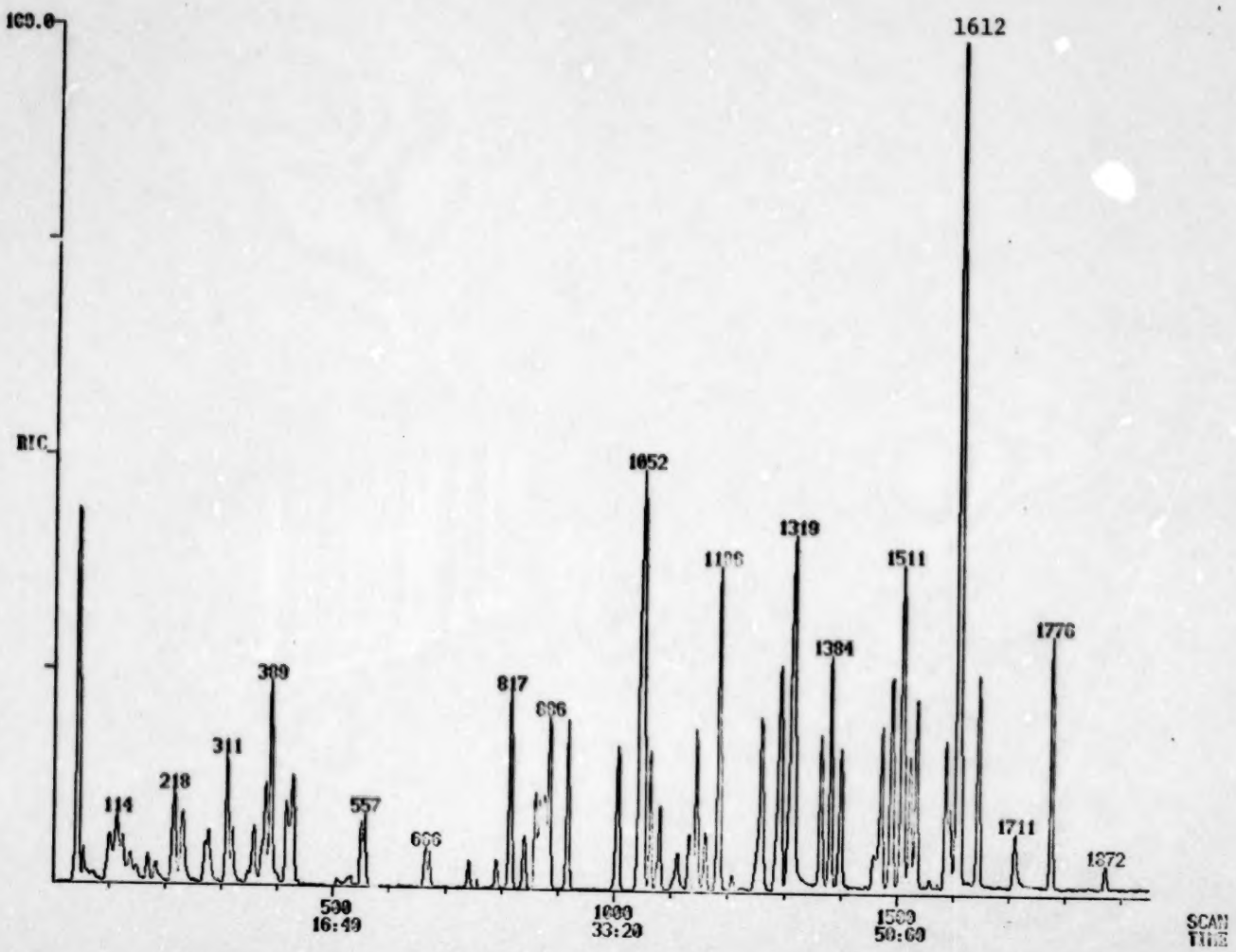

Figure 9. Reconstructed ion chromatogram of mixture containing all chemicals listed in Table 1.

Table 12. DEFINITION OF COMPUTER RANKING IDENTIFICATIONS FOR TABLES IN APPENDIX A

Ranking Value	Description
1	Identification was first choice and correct answer against known composition.
1-	Wrong isomer as first choice.
2	Correct identification was second choice, first choice incorrect.
2-	Wrong isomer as second choice, first choice incorrect.
3	Correct identification was third choice, first and second choices incorrect.
3-	Wrong isomer as third choice, first and second choices incorrect.
4	Correct identification was fourth choice, first, second, third choices incorrect.
4-	Wrong isomer as fourth choice, first, second, third choices incorrect.
5	Correct identification was fifth choice, first, second, third, fourth choices incorrect.
5-	Wrong isomer as fifth choice, first, second, third, fourth choices incorrect.
0	All choices were incorrect.

Note: Manual interpretation has only 1,1-, and 0 possibilities.

Table 13. OVERALL PERCENT CORRECT IDENTIFICATION BY METHOD OF IDENTIFICATION

Method	0	1/-1[a]	2/-2	3/-3	4/-4	5/-5	Missing
Manual	29.3	70.7	-	-	-	-	-
RTI/MSSS							
-D	31.0	59.0	6.0	2.4	1.1	0.5	0
+D	26.8	60.9	7.5	2.8	1.5	0.5	0
MSFS							
-D	42.4	49.5	3.3	2.3	0.9	1.5	0
+D	41.9	48.4	5.0	2.8	0.7	1.3	0
Incos							
-D	21.9	75.2	1.3	0.8	0.3	0.5	0
+D	25.4	58.2	2.0	0.9	0.2	1.1	13.1

[a] See Table 12 for definition.

spectra and with the concentrations of the unresolved components at high or low levels with respect to each other. Furthermore the complexity of the mixtures were gradually increased with each mixture.

Table 14 presents a summary of these design effects on the accuracy of identification. The results in Table 14 again demonstrate that the manual interpretation and the INCOS algorithm appeared to give the highest percent identification accuracy. Again, the worse case was MSFS. In a few cases the application of Rindfleisch deconvolution to raw data appeared to improve the of accuracy of identification, however in most cases there was no significant improvement. As anticipated, higher percent identification accuracy was obtained when the mass spectra were dissimilar for constituents in unresolved chromatographic peaks. An exception to this trend was the results obtained with the MSFS. Finally, for those chromatographic peaks representing triplets, quartets, quintets, and sixtets, the percent accuracy was greater when the constituents were at approximately equivalent concentrations than if they appeared in combinations of high-low concentrations.

The percent correct and incorrect identities by chemical group and method of identification were examined. These results are given in Table 15. (For each chemical class, the search identification routine giving the highest percent correct identification is underlined.) In all cases the identification routines gave the highest accuracy for halogenated alkanes. On the otherhand, the worse results for all cases were observed with aldehydes. For alkanes, alcohols, aldehydes, esters, ethers, nitriles, hydrogen compounds, halogenated alkanes, halogenated aromatics, aromatic aldehydes and acids, the highest percent correct identities were obtained with the INCOS algorithm. For ketones, aromatics, sulfur compounds and phenols, manual identification was superior. In no cases did the MSFS give the best results for any chemical class studied.

The percent correctly identified chemicals by level and method of identification was compared. These results are given in Table 16. From these results it is evident that each chemical is most often correctly identified (regardless of the method of identification) when the concentration of the chemical in a mixture is high. Correspondingly, as the concentration was decreased, the accuracy also likewise decreased. There were some exceptions, however, and these were n-dodecane, n-propyl acetate, di-n-butyl ether,

Table 14. SUMMARY OF DESIGN EFFECT ON PERCENT ACCURACY OF IDENTIFICATION

Design Effect	Manual	RTI/MSSS -D[a]	RTI/MSSS +D	MSFS -D	MSFS +D	Incos -D	Incos +D
Similar Spectra/Medium Level/ Doublet (N=18)[b]	61	55	44	61	39	67	67
Similar Spectra/Hi-Low Level/ Doublet (N=36)	61	58	55	55	50	61	55
Dissimilar Spectra/Medium Level/ Doublet (N=38)	78	66	74	47	60	89	84
Dissimilar Spectra/Hi-Low Level Doublet (N=76)	68	57	67	50	50	84	76
Medium Level/Triplet (N=50)	78	72	66	54	54	72	66
Hi-Low Level/Triplet (N=100)	74	62	64	48	46	80	84
Medium Level/Quartet (N=57)	70	60	65	46	49	75	72
Hi-Low Level/Quartet (N=114)	61	46	53	40	40	66	59
Medium Level/Quintets (N=62)	77	61	68	48	54	77	68
Hi-Low Level/Quintets (N=122)	73	59	53	47	44	78	60
Medium Level/Sextets (N=54)	72	66	67	56	48	76	-[c]
Hi-Low Level/Sextets (N=128)	72	58	58	54	48	72	65

[a] D = deconvolution.

[b] N = number of observations.

[c] Missing data.

Table 15. PERCENT CORRECT/INCORRECT IDENTIFICATION BY CHEMICAL GROUP TYPE AND METHOD OF IDENTIFICATION

Chemical Group	N[a]	Manual	RTIMSSS		MSFS		Incos	
			-D	+D	-D	+D	-D	+D
Alkanes	87							
Correct		74.7	67.8	70.1	6.9	5.7	75.9[b]	59.8
Incorrect		25.3	32.2	29.9	93.1	94.3	24.1	40.2
Alcohols	22							
Correct		40.9	31.8	54.5	45.5	31.8	68.2	73.7
Incorrect		59.1	68.2	45.5	54.5	68.2	31.8	26.3
Aldehydes	42							
Correct		9.5	19.1	31.0	21.4	23.8	14.3	32.4
Incorrect		90.5	80.9	69.0	78.6	76.2	85.7	67.6
Esters	90							
Correct		77.8	70.0	67.8	52.2	57.8	83.3	83.5
Incorrect		22.2	30.0	32.2	47.8	42.2	16.7	16.5
Ethers	45							
Correct		71.1	64.4	68.9	62.2	64.4	82.2	64.1
Incorrect		28.9	35.6	31.1	37.8	35.6	17.8	35.9
Ketones	42							
Correct		81.0	23.8	57.1	28.6	26.2	80.9	73.0
Incorrect		19.0	76.2	42.9	71.4	73.8	19.1	27.0
Nitriles	51							
Correct		33.3	31.4	52.9	31.1	41.2	52.9	35.5
Incorrect		66.7	68.6	47.1	68.9	58.8	47.1	64.5
Nitrogen Compounds	69							
Correct		36.2	30.4	23.2	26.1	17.4	47.8	23.3
Incorrect		63.8	69.6	76.8	73.9	82.6	52.2	76.7
Aromatics	126							
Correct		86.5	78.6	61.9	70.6	64.3	84.1	73.6
Incorrect		13.5	21.4	38.1	29.4	35.7	15.9	26.4

(continued)

Table 15 (cont'd.)

Chemical Group	N	Manual	RTIMSSS		MSFS		Incos	
			-D	+D	-D	+D	-D	+D
Halogenated Alkanes	104							
Correct		95.2	79.8	89.4	84.6	77.6	96.1	91.0
Incorrect		4.8	20.2	10.6	15.4	22.4	3.9	9.0
Halogenated Aromatics	60							
Correct		81.7	75.0	76.7	55.0	70	83.3	80.8
Incorrect		18.3	25.0	23.3	45.0	30	16.7	19.2
Aromatic Aldehydes	15							
Correct		66.7	20.0	40.0	26.7	46.7	86.7	61.5
Incorrect		33.3	80.0	60.0	73.3	53.3	13.3	38.5
Sulfur Compounds	60							
Correct		95.0	71.7	71.7	65.0	60.0	91.7	84.6
Incorrect		5.0	28.3	28.3	35.0	40.0	8.3	15.4
Acids	15							
Correct		26.7	33.3	20.0	33.3	20.0	46.7	30.8
Incorrect		73.3	66.7	80.0	66.7	80.0	53.3	69.2
Phenols	39							
Correct		74.4	79.5	51.3	69.2	53.8	71.8	51.2
Incorrect		25.6	20.5	48.7	30.8	46.2	28.2	48.8

[a]N = number of observations across all mixtures and levels.

[b]Underline = search identification with highest percent correct.

Table 16. PERCENT CORRECT IDENTIFICATION BY CHEMICAL, LEVEL AND METHOD OF IDENTIFICATION

Chemical	Level[a]	N[b]	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
n-Hexane									
	H	2	100	100	100	50	100	100	100
	M	4	50	0	25	0	0	25	33
	L	6	33	33	50	33	33	50	50
n-Heptane									
	H	1	100	100	100	0	0	100	100
	M	5	80	80	100	0	0	100	100
	L	9	56	44	33	22	0	44	38
n-Octane									
	H	-[c]	-	-	-	-	-	-	-
	M	6	50	83	100	17	17	100	60
	L	9	55	44	44	0	0	22	50
n-Decane									
	H	3	100	100	50	0	0	100	100
	M	5	100	80	100	0	0	83	100
	L	8	88	88	75	0	0	100	88
n-Undecane									
	H	2	100	100	100	0	0	100	100
	M	5	60	80	80	0	0	100	75
	L	8	88	75	75	0	0	88	75
n-Dodecane									
	VH	1	100	0	0	0	0	100	0
	H	4	75	75	75	0	0	75	75
	M	5	100	100	100	0	0	80	100
	L	5	80	80	80	0	0	100	75
Methanol									
	H	-	-	-	-	-	-	-	-
	M	1	0	0	0	0	0	0	0
	L	-	-	-	-	-	-	-	-

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Ethanol									
	H	-	-	-	-	-	-	-	-
	M	2	0	0	0	0	25	25	25
	L	4	0	0	0	0	0	0	0
t-Butanol									
	H	1	0	100	50	50	0	50	50
	M	5	60	80	100	80	60	100	80
	L	9	67	78	67	44	33	89	100
Acrolein									
	H	3	0	0	66	0	66	33	66
	M	4	0	0	0	0	0	0	0
	L	5	0	0	0	0	0	0	50
Propionaldehyde									
	VH	1	0	0	0	100	100	100	100
	H	4	50	0	25	50	50	25	25
	M	5	0	0	20	0	20	20	0
	L	5	20	0	0	0	0	0	0
n-Heptaldehyde									
	H	1	100	100	100	100	100	100	100
	M	5	0	80	80	40	20	20	20
	L	9	0	33	44	33	22	0	55
Ethyl acetate									
	H	3	100	100	100	66	100	100	100
	M	4	75	75	75	75	75	80	66
	L	5	60	100	100	100	100	100	80
Methyl methacrylate									
	VH	1	0	100	100	0	0	0	30
	H	4	75	75	75	0	25	75	75
	M	5	80	60	20	0	0	80	75
	L	5	60	60	0	0	0	40	50

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Ethyl acrylate									
	H	1	100	100	100	100	100	100	100
	M	2	50	100	100	100	100	100	100
	L	3	33	100	100	33	100	100	100
n-Propyl acetate									
	H	4	75	75	75	75	75	75	100
	M	5	100	100	100	83	83	83	100
	L	7	71	100	100	71	57	100	100
n-Butyl acetate									
	VH	1	100	100	100	100	100	0	0
	H	4	100	100	100	100	100	75	100
	M	5	80	100	83	80	100	80	100
	L	5	60	40	100	80	100	80	100
n-Butyl acrylate									
	H	3	100	100	100	100	100	100	66
	M	4	100	75	50	50	75	75	66
	L	5	60	60	60	40	40	80	40
n-Butyl methacrylate									
	H	1	100	0	0	0	0	50	50
	M	5	100	20	20	0	0	100	100
	L	9	78	22	0	0	0	67	100
Diethyl ether									
	H	-	-	-	-	-	-	-	-
	M	1	0	0	0	0	0	0	0
	L	2	0	0	0	0	0	50	100
Methyl furan									
	H	2	100	100	100	100	100	100	100
	M	6	100	33	17	83	83	100	100
	L	10	90	70	70	50	60	100	56

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Di-n-butyl ether									
	H	1	0	0	0	0	0	0	0
	M	3	0	66	33	0	0	33	0
	L	5	100	40	60	20	20	40	20
2-Methylbenzofuran									
	VH	1	100	0	0	0	0	0	0
	H	4	100	100	100	100	100	100	100
	M	5	100	100	100	100	100	100	75
	L	5	100	100	100	100	100	100	100
2-Pentanone									
	VH	1	100	0	0	0	0	100	100
	H	5	100	40	60	0	0	100	100
	M	6	100	33	83	17	0	83	80
	L	6	100	17	67	33	0	100	80
3-Pentanone									
	H	1	100	100	100	100	100	100	100
	M	3	66	66	100	100	100	100	100
	L	5	100	100	100	100	100	100	100
Acetone									
	H	1	100	0	100	0	0	50	50
	M	5	100	0	40	0	20	60	25
	L	9	22	0	0	0	11	44	38
Acetonitrile									
	H	3	0	0	0	0	0	0	0
	M	5	0	0	0	0	0	0	0
	L	7	0	0	14	0	14	0	0
Acrylonitrile									
	H	2	100	100	50	100	100	100	50
	M	3	33	0	100	0	33	0	100
	L	4	0	25	25	0	0	25	0

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
α-Methylbutyronitrile									
	H	3	33	100	100	100	66	75	75
	M	4	25	25	25	50	50	100	40
	L	5	0	0	20	0	17	80	20
Benzonitrile									
	H	1	100	100	100	100	100	100	100
	M	5	100	80	80	60	80	100	50
	L	9	67	44	78	33	78	78	50
Pyridine									
	H	1	0	0	0	0	0	50	-
	M	6	100	100	100	83	67	83	80
	L	8	62	50	25	50	33	87	50
Nitrobenzene									
	H	1	100	100	100	100	100	100	100
	M	5	100	80	80	80	60	80	75
	L	9	55	44	22	44	22	89	12
Piperidine									
	VH	1	100	0	0	0	0	0	0
	H	4	0	0	0	0	0	0	0
	M	5	0	0	0	0	0	0	0
	L	5	0	0	0	0	0	0	0
Pyrrolidine									
	H	3	0	0	0	0	0	0	0
	M	4	0	0	0	0	0	0	33
	L	5	0	0	0	0	0	0	0
Quinoline									
	H	2	100	50	50	0	0	100	0
	M	4	25	0	0	0	0	100	0
	L	6	0	0	0	0	0	100	-

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Benzene									
	H	7	100	57	100	100	86	100	100
	M	-	-	-	-	-	-	-	-
	L	8	87	62	87	50	100	100	100
Toluene									
	H	2	100	100	100	100	100	100	100
	M	5	100	100	100	100	100	100	100
	L	8	87	87	87	75	75	100	100
o-Xylene									
	H	2	100	100	100	100	100	100	100
	M	4	100	100	100	100	100	100	100
	L	6	100	33	83	33	50	83	50
m-Xylene									
	H	1	100	100	100	100	100	100	100
	M	1	0	100	100	100	100	100	100
	L	1	100	100	100	100	100	100	100
p-Xylene									
	H	1	0	0	0	0	0	0	0
	M	1	0	0	0	0	0	0	0
	L	1	0	0	0	0	0	0	0
m-Ethyltoluene									
	VH	1	100	0	0	0	0	100	0
	H	5	100	20	20	60	40	100	40
	M	7	86	86	67	67	33	67	60
	L	6	83	67	33	50	50	83	20
1,3,5-Trimethylbenzene									
	VH	1	100	0	0	50	50	50	0
	H	4	75	100	100	100	100	100	100
	M	5	40	100	60	100	60	100	75
	L	6	60	100	80	80	80	100	100

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Naphthalene									
	VH	1	100	0	0	0	0	0	0
	H	4	100	25	25	50	50	100	100
	M	5	100	100	25	40	80	100	75
	L	5	100	60	60	100	40	80	75
Styrene									
	VH	1	100	0	0	100	100	100	100
	H	4	100	100	100	100	100	100	100
	M	5	100	100	100	100	100	80	100
	L	5	100	100	100	100	100	100	100
Methyl bromide									
	H	1	100	100	100	100	100	100	100
	M	-	-	-	-	-	-	-	-
	L	-	-	-	-	-	-	-	-
Vinyl chloride									
	H	2	100	100	100	100	100	100	100
	M	4	100	75	100	100	100	100	100
	L	6	100	50	83	67	67	100	67
Methylene chloride									
	VH	1	100	100	100	100	100	100	100
	H	4	100	100	100	100	25	100	100
	M	5	100	100	100	20	60	100	100
	L	5	100	100	100	80	20	100	100
1,1,1-Trichloroethane									
	H	2	100	100	100	100	100	100	100
	M	4	100	25	100	100	100	100	100
	L	5	83	0	67	50	50	100	67
1,2-Dichloroethane									
	H	6	80	100	100	100	100	100	100
	M	-	-	-	-	-	-	-	-
	L	9	78	78	78	78	89	89	78

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
1,2-Dichloropropane									
	H	2	100	100	100	100	100	100	83
	M	4	100	75	100	100	100	100	100
	L	6	100	100	67	100	100	100	100
Tetrachloroethylene									
	H	2	100	100	100	100	100	100	100
	M	4	100	100	100	100	100	100	75
	L	6	83	100	100	83	83	67	83
Chloroform									
	H	-	-	-	-	-	-	-	-
	M	2	100	100	100	50	50	100	100
	L	4	100	50	50	75	25	100	75
1,1,2,2-Tetrachloroethane									
	H	-	-	-	-	-	-	-	-
	M	1	100	100	100	100	100	100	100
	L	2	100	100	100	100	100	100	100
Hexachlorobutadiene									
	H	1	100	100	100	100	100	100	100
	M	6	83	83	83	83	83	83	100
	L	9	100	100	100	100	100	100	100
p-Dichlorobenzene									
	VH	1	100	0	0	100	100	0	0
	H	4	100	100	100	100	100	100	100
	M	5	100	100	100	100	100	100	100
	L	5	100	100	100	80	80	100	100
Perfluorobenzene									
	VH	1	100	100	100	100	100	100	100
	H	4	100	75	75	75	75	100	75
	M	8	100	100	100	100	100	100	100
	L	5	40	0	20	0	20	40	25

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
Perfluorotoluene									
	VH	1	100	100	100	100	100	100	100
	H	4	100	75	100	75	75	75	100
	M	6	83	66	83	33	33	100	100
	L	4	80	20	80	20	20	100	100
o-Chloronitrobenzene									
	VH	1	100	0	0	100	100	100	100
	H	4	75	75	75	50	75	100	100
	M	5	20	0	20	0	0	40	20
	L	5	80	0	80	100	80	60	40
p-Tolualdehyde									
	VH	1	100	0	0	100	100	100	0
	H	4	75	25	75	75	75	100	100
	M	5	40	0	40	0	20	20	40
	L	5	80	0	20	0	0	80	40
Thiophene									
	VH	1	100	100	100	100	100	100	100
	H	4	100	100	100	0	0	100	100
	M	5	100	100	100	20	20	100	100
	L	5	100	100	100	20	0	100	100
2-Methylthiophene									
	VH	1	100	0	0	0	100	100	0
	H	4	100	100	100	100	100	100	100
	M	5	100	100	100	80	80	80	100
	L	5	100	40	100	100	100	100	100
1-Benzothiophene									
	H	2	100	100	100	100	100	100	50
	M	5	100	100	100	100	100	100	100
	L	8	100	100	100	100	100	100	100

(continued)

Table 16 (cont'd.)

Chemical	Level	N	Manual	RTIMSSS		MSFS		Incos	
				-D	+D	-D	+D	-D	+D
2-Benzothiazole									
	H	2	100	0	0	100	50	100	50
	M	5	100	0	0	60	40	80	20
	L	8	62	0	0	38	12	62	62
Acetic acid									
	H	1	0	0	0	0	0	0	0
	M	5	0	20	0	20	0	40	0
	L	9	44	44	33	44	33	55	44
m-Cresol									
	H	3	100	66	66	66	33	66	33
	M	5	20	60	20	60	20	60	60
	L	7	14	43	0	14	14	43	28
p-Cresol									
	H	3	100	100	100	100	66	33	66
	M	4	100	100	100	100	100	50	50
	L	5	100	80	80	100	100	100	80
Phenol									
	H	2	100	100	0	100	100	100	100
	M	4	100	100	75	75	50	100	100
	L	6	100	100	50	66	50	100	33
Vinyl bromide									
	H	1	100	100	100	100	100	100	100
	M	-	-	-	-	-	-	-	-
	L	-	-	-	-	-	-	-	-

[a]See Tables 11 for concentration level in mixture.

[b]N = number of observations across all mixtures and levels.

[c]No data at this level.

2-methylbenzofuran, pyridine, m-ethyltoluene, trimethylbenzene, naphthalene, 2-methylthiophene, and acetic acid. In these cases when the levels were either high or very high the identification routines failed more frequently to identify the chemicals correctly. As previously indicated these results in Table 16 also indicate that the MSFS had extreme difficulty in properly identifying any of the alkanes.

An overall comparison was also made of the percent correct and incorrect identifications between manual and the computer algorithm methods. These results are shown in Table 17. The combination of manual identification and INCOS algorithm on raw data (nondeconvoluted) yielded the highest agreement (63.6%), i.e. when both approaches correctly identified the same chemical. The lowest percentage agreement observed was for manual and deconvoluted data using the MSFS (43.0%).

A 2 x 2 comparison was also made between computer identification algorithms to determine the percent that both methods gave either correct or incorrect results (Table 18). The highest agreement (55.3%) was between Incos (nondeconvoluted data) and RTI/MSSS (deconvoluted data). Similarly the worst agreement was with MSFS. Finally a comparison between raw data (nondeconvoluted) and deconvoluted data using the INCOS algorithm is also shown. Surprisingly the agreement was only 61.6%, i.e. when both correctly identified the analytes.

Table 17. COMPARISON OF PERCENTAGE CORRECT AND INCORRECT IDENTIFICATIONS BETWEEN MANUAL AND COMPUTER IDENTIFICATION METHODS

		RTIMSSS			
		-D		+D	
		Correct	Incorrect	Correct	Incorrect
Manual	Correct	52.6% (456)[a]	18.1% (157)	53.2% (461)	17.5% (152)
	Incorrect	6.5% (56)	22.8% (198)	7.7% (67)	21.6% (187)

		MSFS			
		-D		+D	
		Correct	Incorrect	Correct	Incorrect
Manual	Correct	45.1% (391)	25.6% (222)	43.0% (373)	27.7% (240)
	Incorrect	4.4% (38)	24.9% (216)	5.4% (47)	23.9% (207)

		INCOS			
		-D		+D	
		Correct	Incorrect	Correct	Incorrect
Manual	Correct	63.6% (551)	7.2% (62)	57.2% (431)	13.2% (99)
	Incorrect	11.6% (101)	17.6% (153)	9.8% (74)	19.8% (149)

[a]Number of observations.

Table 18. COMPARISON OF PERCENTAGE CORRECT AND INCORRECT IDENTIFICATIONS BETWEEN COMPUTER IDENTIFICATION ALGORYTHYMS

		RTIMSSS			
		-D		+D	
		Correct	Incorrect	Correct	Incorrect
INCOS (-D)	Correct	53.4% (463)	21.7% (189)	55.3% (479)	20.0% (173)
	Incorrect	5.7% (49)	19.2% (166)	5.6% (49)	19.1% (166)

		MSFS			
		-D		+D	
		Correct	Incorrect	Correct	Incorrect
INCOS (-D)	Correct	45.9% (398)	29.3% (254)	44.4% (385)	30.8% (267)
	Incorrect	3.6% (31)	21.2% (184)	4.0% (35)	20.8% (180)

		INCOS			
				+D	
				Correct	Incorrect
INCOS (-D)			Correct	61.6% (464)	13.3% (100)
			Incorrect	5.4% (41)	19.7% (148)

SECTION 5

ENVIRONMENTAL SAMPLES

INTRODUCTION

To further test the computer algorithms' ability to identify organic compounds, environmental ambient air samples were collected. Even though synthetic mixtures were used to evaluate the search algorithms, they do not necessarily represent the level of complexity that might be encountered with environmental samples, since environmental samples may contain several hundred constituents in various concentration ratios. However, the synthetic mixtures allowed a true method of assessing the accuracy of identification, since the composition of the mixtures were exactly known. With environmental samples the composition is totally unknown and thus the comparison of identification can only be on a relative basis, e.g. to manual interpretation.

The two algorithms that were further examined were the RTI/MSSS and the INCOS system. The MSFS was not included in this portion of the study since it performed so poorly with synthetic mixtures.

A number of criteria were used to select a candidate list of sites. A primary objective was to achieve a broad based validation and assessment which spanned the spectrum of chemical classes. The criteria for selecting sites were: (1) the chemical classes potentially emitted because of the particular industrial activities; (2) the potential emission rates were of sufficient magnitude to provide significant measurable levels in the ambient air; (3) the assessibility of sites to locating sampling systems; (4) the presence of dense populations near the chemical industry, and (5) the potential for a unique background or interferences to the qualitative analysis by GC/MS/COMP.

This section presents the results of the application of manual and computer algorithms to the identification of chemicals detected in environmental ambient air samples.

EXPERIMENTAL PROCEDURES

Sites Selected, Sampling Design and Sampling

To collect samples with certain classes of volatile organic compounds present, a series of field trips were undertaken. Table 19 presents the seven sites selected for the collection of vapor-phase organics. Environmental samples from these sites presented the opportunity to sample ambient air containing nitrogenous substances, halogenated hydrocarbons, mercaptans, petroleum hydrocarbons and aromatics, acrylonitrile, alkylated leads and other industrial chemicals.

The sampling and analysis methods employed in this study have been previously described (6). The strategy for air sampling is given in Table 20. Three samples were taken, each in triplicate. Two locations were used at each site with one location used to collect a high and low volume sample (25 and 5 ℓ, respectively) over a period of ~25 min. Locations were always selected using meteorological considerations so that each location was generally downwind from the industrial facility. Short sampling times were employed to minimize the effects of erratic meteorological conditions such as wind direction.

Table 21 presents the specific parameters of the environmental sites sampled. The site, location, date of sampling and the general description of the meterological conditions are given.

Sample Analysis by GC/MS and Data Processing

The analysis of environmental ambient air samples collected on Tenax GC cartridges, blanks (sampling cartridges taken to the field and returned unused) and controls (Tenax cartridges spiked with selected chemicals from the list for synthetic mixtures were taken to the field and returned) were analyzed by high resolution GC/MS as previously described (6). The gas chromatographic operating conditions were identical to those given in Table 3. The analysis of field collected samples at each site was completed within 3 weeks after their collection. In addition to the samples collected, three controls and three blank Tenax cartridges were analyzed for quality assurance purposes. The controls were prepared using the chemicals listed in Table 4 on cartridge No. 1. Two replicates of each sample, the field blanks and controls, were spiked with perfluorobenzene and perfluorotoluene as external standards before analysis by GC/MS.

Table 19. ENVIRONMENTAL SITES SELECTED FOR COLLECTION OF VAPOR-PHASE ORGANICS

Site No.	Site	Industry	Chemicals
1	Deepwater, NJ	E.I. DuPont de Nemours & Co., Inc.	Nitrogenous substances
2	Plaquemine, LA	Dow Chemical Corp.	Halogenated hydrocarbons
3	Beaumont, TX	Pennwalt Corp. Mobil Oil Corp.	Mercaptans Petroleum refining
4	Beaumont, TX	E.I. DuPont de Nemours & Co., Inc. PPG Industries	Acrylonitrile, T.E.L. Tetramethyl & Tetraethyllead
5	Lake Charles, LA	PPG Industries	Halogenated hydrocarbons
6	Port Neches, TX	Texaco Chemical	Industrial Chemicals
7	Port Arthur, TX	Gulf Oil Corp. Texaco (Great Lakes Carbon Corp.)	Crude Oil processing Petroleum, coke

Table 20. PARAMETERS FOR AIR SAMPLING

Sample No.	No. of Replicates	Location	Flow Rate	Total Sampling Time (min)	Total Volume (L)
1	3	1	1 L/min	25	25
2	3	1	200 mL/min	25	5.0
3	3	2	1 L/min	25	25

Table 21. SPECIFIC PARAMETERS OF THE ENVIRONMENTAL SITES SAMPLED

Site No.	Location No.	Date Sampled	Description of Location	Description of wind direction and speed	Temp (°F)	Comments
1	1	2/4/83	Approx. 0.8 mi N of NJ turnpike on Rt 130	Esterly at approx. 20 mph (quoting)	36	Faint odor similar to esters
	2	2/4/83	Approx. 0.3 mi N of NJ turnpike and 0.1 mi W of Rt 130	(same)	(same)	(same)
2	1	5/13/83	Approx. 1 mi. W of Rt 1 on Rt 1148	Easterly at 5-10 mph	102	No noticeable odors
	2	5/13/83	Approx. 1 mi. N on Rt. 1 from intersection of Rt. 1148	(same)	93	(same)
3	1	6/28/83	Approx. 50 yds W of entrance to Penwalt	Southerly at ~10 mph	90	Refinery odor; no mercaptans noticed
	2	6/28/83	Approx. 10 yds. from Penwalt plant prop. - downwind	(same)	(same)	(same)
4	1	6/28/83	In Spindletop Park ~2 mi N of DuPont plant	Westerly and Southwesterly winds at ~10 mph	89	Occasional chemical odor noticed
	2	6/28/83	(same)	(same)	(same)	(same)
5	1	6/29/83	Approx. 150 yds from plant entrance - near I-10 - downwind	Southwesterly at ~15 mph slight gusts with precipitation	85	Chemical odor
	2	6/29/83	Beside plant prop. due N of plant	Westerly to Northwesterly winds - 5-10 mph; heavy precipitation for 15 min; variable wind dir.	82	No odors noticed

(continued)

Table 21 (cont'd.)

Site No.	Location No.	Date Sampled	Description of Location	Description of wind direction and speed	Temp (°F)	Comments
6	1	6/29/83	Approx. ~1/4 mi NW of plant - off of Rt 366 at Orchard Ave.	Westerly (steady) at ~15 mph	91	Chemical odors
	2	6/29/83	Due W of plant off of Rt 366 (beside plant prop.)	Westerly at 10-15 mph	90	(same)
7	1	6/30/83	Between Gulf and Texaco plants - downwind of Gulf (on Rt 214)	Westerly and gusting at ~20-25 mph	88	Strong refinery odor; heavy truck traffic
	2	6/30/83	NE of Texaco off of Rt 73 approx ~1/4 mi. W of Savannah Ave.	West southwesterly winds at ~20-25 mph	90	Occasional chemical odor

Again the data acquired was stored on hard disk and magnetic tape for further processing by each of the identification algorithms. The raw and deconvoluted data were subjected to the RTI/MSSS and INCOS systems to identify the chemicals in each of the environmental samples. Also a skilled research investigator interpretated the raw mass spectral data to identify the constituents present in the samples. To perform this, each individual scan from the GC run was printed in bar graph form by means of the commerical GC/MS computer processing programs provided with each mass spectrum data acquisition system. In addition the total ion current plot for each run was computed and presented graphically as an aid to the manual interpretation of the data. The analyst was provided with extensive tables of mass spectral data libraries available both in bar graph and numeric form as well as the Eight Peak Index of Mass Spectral Data (7), however, retention times were not employed to assist in identification of chemicals. Furthermore, the analyst had an extensive list of compounds previously identified in environmental samples arranged in sequence according to elution time characteristics.

Statistical Analysis

Statistical analysis was performed to test the comparability of the different identification routines of compound identification and to identify which factors (e.g., Rindfleisch deconvolution), if any, affect their comparability.

For example a particular sample of N compounds were manually identified, assumed correct and denoted as C_1, C_2, etc. to C_N. For automated procedure J (e.g. the INCOS automated procedure) suppose T_j compounds were identified and that a 1 was recorded for each compound in the manually identified set of compounds which had a match among the compounds identified by the automated procedure and a 0 if there was no match. Then for each sample a matrix of matches (1's or 0's) were formed as in Table 22. Table 22 shows how the matrix of matches by automated method for a particular sample was constructed.

Continuing in Table 22, $X_i = 1$ if compound k of the manual procedure had a match in automated procedure (1) and $X_k = 0$ if compound k had no match. Similarly, Y_k and Z_k were defined and, therefore, the totals ΣX_i, ΣY_i, and ΣZ_i were simply the number of times the automated procedure matched the manual procedure in the sample. Dividing these totals by the number of manually

Table 22. **MATRIX OF MATCHES BY AUTOMATED METHOD - SAMPLE A**

Compounds Identified Manually		Automated Methods* (1)	(2)	(3)	...
C_1		X_1	Y_1	Z_1	
C_2		X_2	Y_2	Z_2	
C_3		X_3	Y_3	Z_3	
.		.	.	.	
.		.	.	.	
.		.	.	.	
C_N		X_N	Y_N	Z_N	
	Total Matches	ΣX_i	ΣY_i	ΣZ_i	
	Total Compounds Identified				
N		T_1	T_2	T_3	...

*(1) = RTI raw spectra with custom spectral library search.
(2) = RTI clean spectra (Rindfleisch deconvolution) with custom spectral library search.
(3) = INCOS automated method with standard spectral search.

identified compounds (N) gave $\hat{P}_{1A}$, $\hat{P}_{2A}$, $\hat{P}_{3A}$, the estimated probabilities of a match with the manually identified compounds on a sample.

The same tabulation for each of the 12 air samples was performed to give a 12 x 4 matrix of estimated probabilities denoted as $\hat{P}$.

RESULTS AND DISCUSSION

Since the correct answer on the identification of the chemicals in the environmental ambient air samples could not be known, then the only comparison that could be made was relative to manual interpretation. Thus, all of the results presented in this section are relative to the skilled interpretators evaluation of the data. The results of the manual interpretation and the agreement between the results obtained from the computer algorithms and manual interpretation are given in Appendix B. After examining the reconstructed ion current chromatograms for each of the samples analyzed by GC/MS, 13 were selected for data analysis. Of these 1 sample collected at Site No. 3 was lost because of a computer malfunction. Thus the results presented are for 12 environmental samples collected at each of six sites. In some cases e.g. Site 1, 2, 4 and 6, either more than one location or a combination of high/low air volumes were selected for comparative purposes.

To provide a general perspective of the complexity of the environmental air samples, Figures 10 to 12 are shown. Inspection of the chromatographic peaks and the general baseline reveals that considerable convolution of components still remain after gas chromatography of these mixtures. This was the case for most of the environmental air samples analyzed, and were typical in complexity as experienced in other studies (9). Therefore, these samples were belived to present the typical problems generally encountered in identifying substances.

Table 23 presents the percent agreement overall and by chemical class observed in these environmental air samples between manual and automated procedures. The greatest percent agreement occurred between manual and deconvoluted data interpreted by the INCOS system. However, this agreement was only 53.9%. The percentage agreement by chemical class is also given, however the number of observations in some cases was rather small (e.g. chemical classes 7, 8 and 13). In general the Incos automated method agreed more often by chemical class with manual than RTI/MSSS.

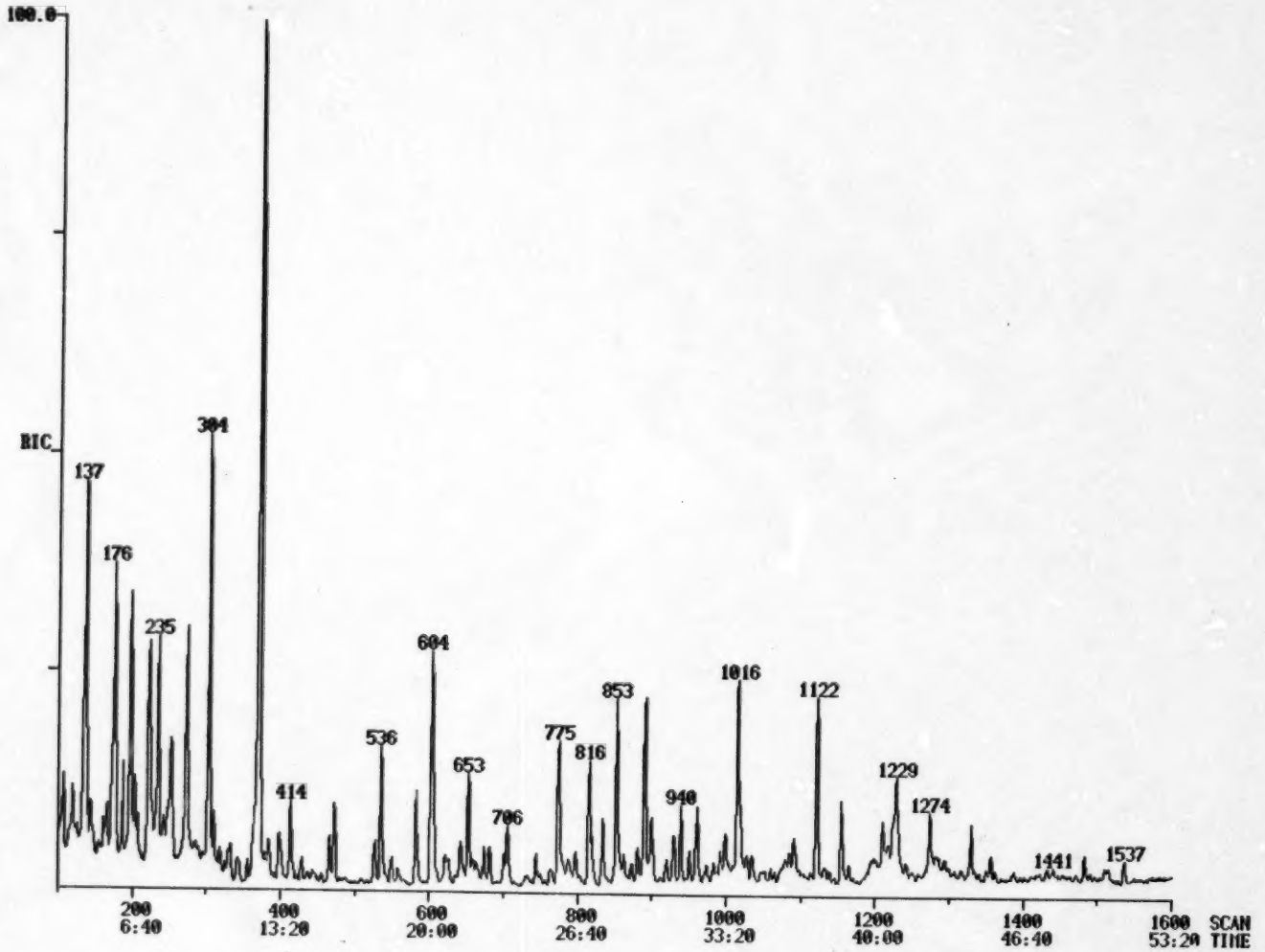

Figure 10. Reconstructed ion chromatogram for ambient air sample from site No. 1, location No. 1 (hi volume, see Table 21).

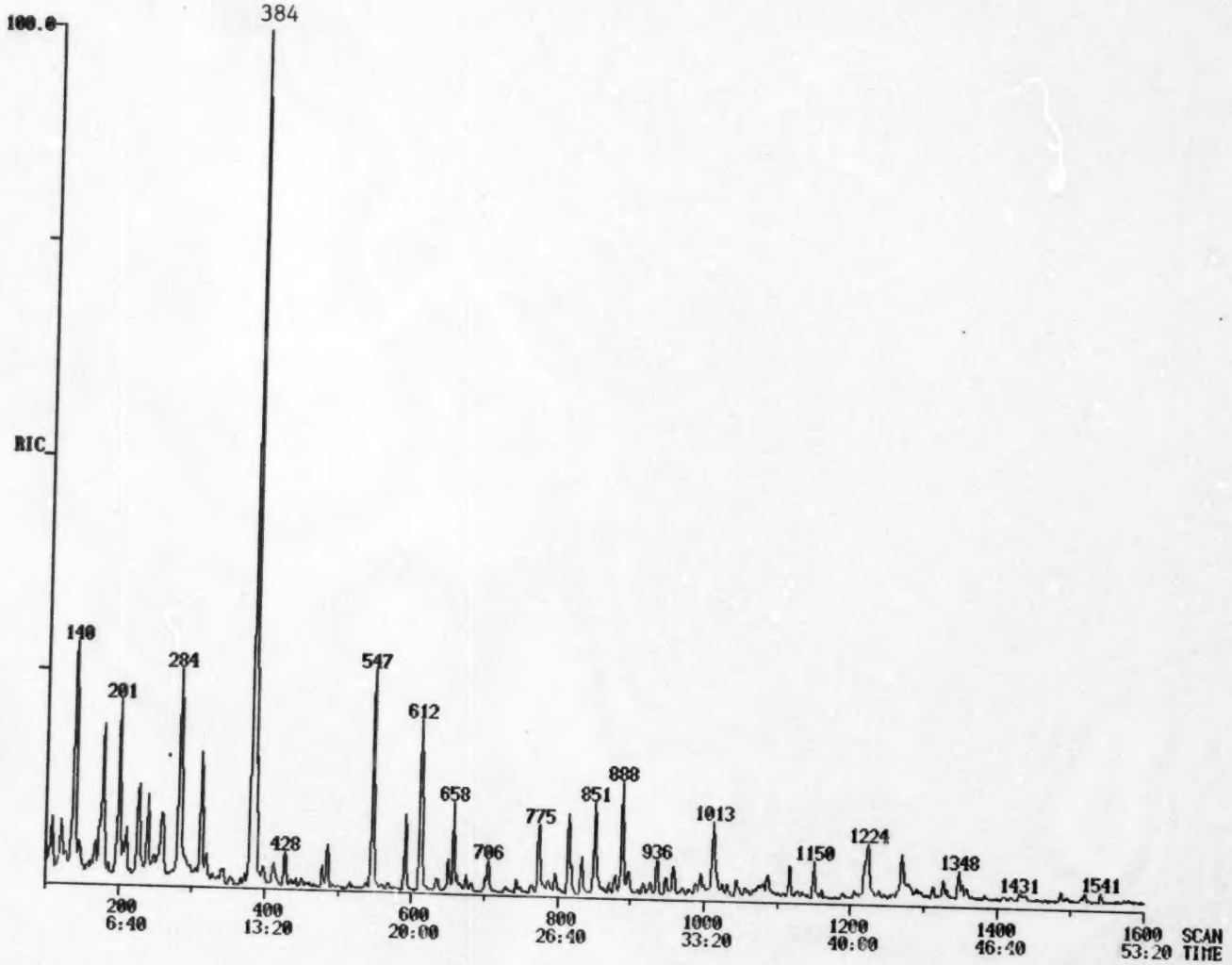

Figure 11. Reconstructed ion chromatogram for ambient air sample from site No. 1, location No. 2 (hi volume, see Table 21).

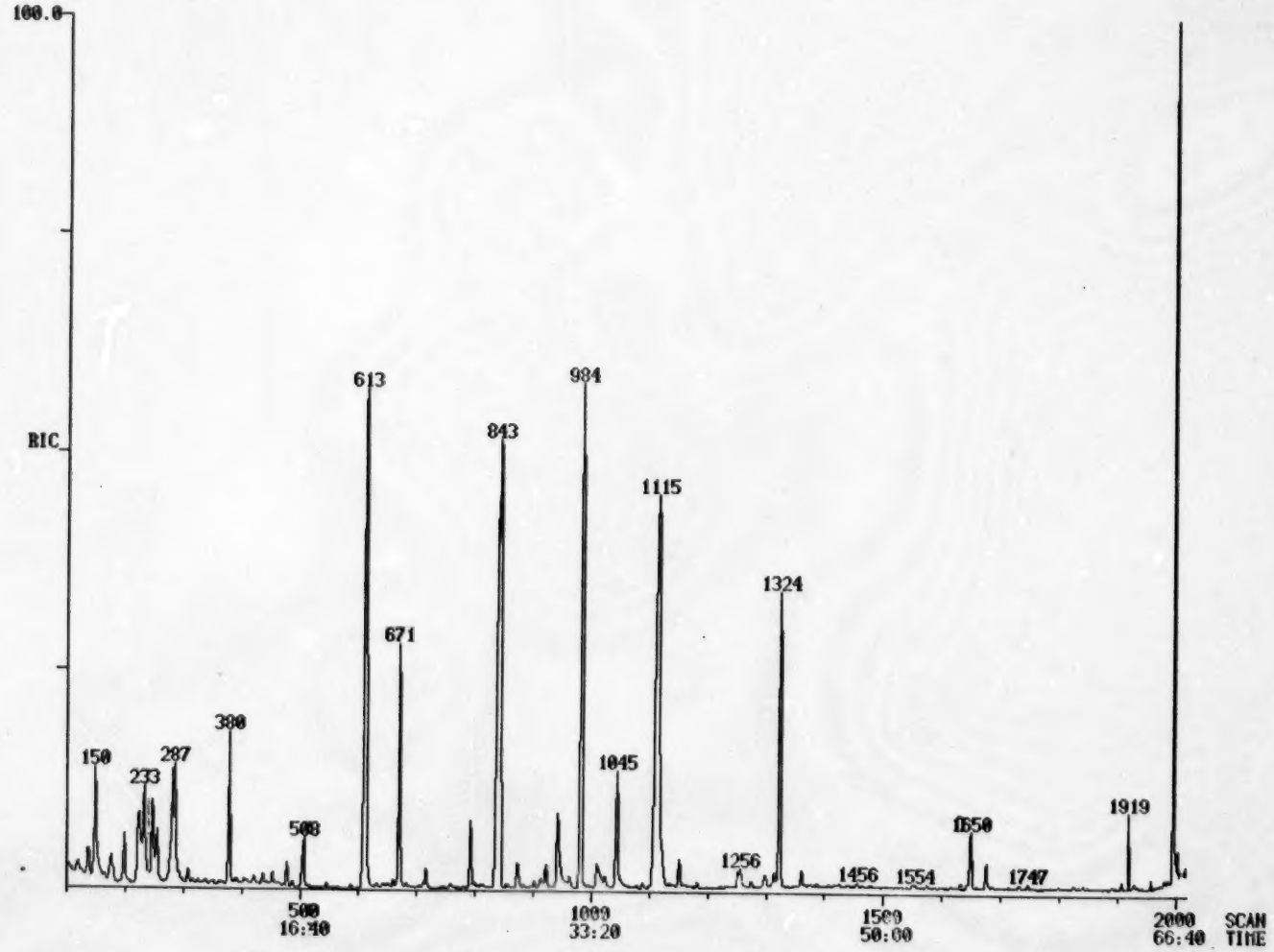

Figure 12. Reconstructed ion chromatogram for ambient air sample from site No. 2, location No. 1 (low volume, see Table 21).

Table 23. PERCENT AGREEMENT OVERALL AND BY CHEMICAL CLASS[a]

Chemical Class	Overall (997)[b]	RTI MSSS		INCOS	
		-D	+D	-D	+D
		49.8	44.3	47.6	53.9
1	(458)	46.7	43.5	39.7	50.4
2	(14)	21.4	21.4	78.6	50.0
3	(24)	70.8[c]	62.5	66.7	70.8
4	(44)	47.7	45.5	61.4	52.3
5	(15)	40.0	46.7	40.0	46.7
6	(20)	40.0	35.0	70.0	60.0
7	(5)	20.0	100.0	40.0	100.0
8	(8)	75.0	62.5	25.0	50.0
9	(229)	55.0	45.0	47.2	56.8
10	(59)	47.5	39.0	42.4	67.8
11	(36)	83.3	77.8	88.9	69.4
12	(13)	30.8	7.7	84.6	84.6
13	(5)	0	20.0	40.0	0
14	(16)	43.8	37.5	68.8	43.8
15	(51)	51.0	47.1	51.0	45.1

[a]With manual.

[b]Sample size.

[c]Underline = highest percent correct for chemical class.

The percentage agreement between the identification routines was ranked and is given in Table 24. Both the RTI/MSSS and INCOS had the highest percentage agreement with manual identification for raw data on halogenated aromatics. Interestingly both systems also had the highest percentage agreement with deconvoluted data on nitriles. The trends, however, were not similar for the remaining chemical classes when comparing the RTI/MSSS and INCOS with manual interpretation. The highest agreement was between INCOS and manual interpretation for all of the chemical classes. These observations appear to be consistent with those obtained with synthetic mixtures.

The results of the data for environmental ambient air samples were sorted and compared to determine the percent agreement by environmental sample. These data are presented in Table 25. Interestingly a higher percentage agreement with manual interpretation was observed with the RTI/MSSS on raw data with site 1 for locations 1 and 2 whereas the reverse was the case in a couple of instances on deconvoluted data. With the remaining sites and locations, the percent agreement was higher between manual and INCOS search system on raw data and deconvoluted data.

Finally the data was sorted and examined to determine the percent agreement by site and the same location for different volumes of environmental air that was sampled. These data are given in Table 26. For the RTI/MSSS algorithms, the higher volume of air sampled (and therefore higher absolute levels of chemicals collected on the Tenax GC cartridge) gave the higher agreement with manual interpretation for raw data. The trend appeared to be reverse when the data were deconvoluted, i.e. the percent agreement decreased in many cases.

In contrast to the synthetic mixtures that were analyzed, the RTI/MSSS performed better with the environmental samples and appeared to agree as well as the INCOS search system relative to manual interpretation.

Table 24. PERCENT IN AGREEMENT RANKED BY AUTOMATED PROCEDURE

	RTI MSSS				INCOS			
	-D		+D		-D		+D	
Rank	% Agree	Class	% Agree	Class	% Agree	Class	% Agree	Class
1	83.3	11	100.0	7	88.9	11	100.0	7
2	75.0	8	77.8	11	84.6	12	84.6	12
3	70.8	3	*62.5	3	78.6	2	70.8	3
4	55.0	9	*62.5	8	70.0	6	69.4	11
5	51.0	15	47.1	15	68.8	14	67.8	10
6	47.7	4	46.7	5	66.7	3	60.0	6
7	47.5	10	45.5	4	61.4	4	56.8	9
8	46.7	1	45.0	9	51.0	15	52.3	4
9	43.8	14	43.5	1	47.2	9	50.4	1
10	*40.0	5	39.0	10	42.4	10	*50.0	2
11	*40.0	6	37.5	14	*40.0	5	*50.0	8
12	30.8	12	35.0	6	*40.0	7	46.7	5
13	21.4	2	21.4	2	*40.0	13	45.1	15
14	20.0	7	20.0	13	39.7	1	43.8	14
15	0	13	7.7	12	25.0	8	0	13

*Ties.

Class 3 and 11 are common to top 6 of all methods. Class 13 is common to bottom 3.

Table 25. PERCENT AGREEMENT BY SAMPLE (SITE AND LOCATION)

Sample			RTI MSSS		INCOS	
Site	Location	N	-D	+D	-D	+D
1	1	165	63.6	42.4	38.2	59.4
1	2	114	66.7	68.4	31.6	66.7
2	1	146	63.7	50.7	41.8	69.2
2	2	82	63.4	53.7	48.8	67.1
4	1	161	31.1	31.1	57.8	34.2
5	1	35	25.7	20.0	60.0	28.6
6	1	104	39.4	46.2	51.0	48.1
6	2	91	27.5	30.8	57.1	38.5
7	2	99	46.5	43.4	56.6	57.6

Table 26. PERCENT AGREEMENT BY SITE AND SAME LOCATION FOR DIFFERENT VOLUMES

				% Agreement			
				RTIMSSS		INCOS	
Site	Loc	Volume	N	-D	+D	-D	+D
1	1	High	95	68.4	37.9	34.7	58.9
	1	Low	70	57.1	48.6	42.9	60.0
2	1	High	76	72.4	44.8	44.7	72.4
	1	Low	70	54.3	57.1	38.6	65.7
4	1	High	94	34.0	28.7	54.3	33.0
	1	Low	67	26.9	34.3	62.7	35.8

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APPENDIX A

SUMMARY OF RESULTS FOR EACH MIXTURE SUBJECTED TO MANUAL AND AUTOMATED ALGORITHM IDENTIFICATION

Table A1. CHEMICALS IDENTIFIED IN MIXTURE NO. 1

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	M[g]	0	0	0	0	0	0	0
Acetonitrile	7	M	0	0	0	0	0	0	0
2-Methylfuran	5	M	1	1-	3-	1-	2-	1	1
Ethyl acetate	4	M	1	1	1	1	1	1	1
Pyrrolidine	8	M	0	0	0	0	0	0	0
2-Pentanone	6	M	1	1-	1	2	3	1	1
3-Pentanone	6	M	1	0	1	1	1	1	1
Ethyl acrylate	4	M	1	1	1	1	1	1	1
n-Propyl acetate	4	M	1	1	1	1	0	1	1
α-Methylbutyronitrile	7	M	1	1	0	1	1-	1	1-
m-Xylene	9	M	0	1	1-	1	1	1-	1
p-Xylene	9	M	0	0	0	0	0	0	0
Di-n-butyl ether	5	M	0	0	0	0	0	0	0
n-Butyl acrylate	4	M	1	1	1	1	1	1	1
m-Ethyltoluene	9	M	1	1-	2-	1	2	1	1
p-Ethyltoluene	9	M	1	0	0	1	0	1-	1
p-Cresol	15	M	1	1-	1-	1	1	1-	1-
m-Cresol	15	M	0	0	0	0	0	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A2. CHEMICALS IDENTIFIED IN MIXTURE NO. 2

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	H[g]	0	0	0	0	0	0	0
Acetonitrile	7	L	0	0	0	0	0	0	0
2-Methylfuran	5	H	1	1-	1-	1-	1-	1	1
Ethyl acetate	4	L	1	1	1	1	1	1	1
Pyrrolidine	8	H	0	0	0	0	0	0	0
2-Pentanone	6	L	1	1-	1	1	0	1	2
3-Pentanone	6	H	1	0	1	1	1	1	1
Ethyl acrylate	4	L	0	0	1	0	1	1	1
n-Propyl acetate	4	H	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	L	0	0	0	0	0	1	0
m-Xylene	9	H	1	1	1	1	1	1-	1-
p-Xylene	9	L	0	0	0	0	0	0	0
Di-n-butyl ether	5	H	0	0	0	0	0	0	0
n-Butyl acrylate	4	L	1	1	1	1	1	1	1
m-Ethyltoluene	9	H	1	1	1-	1	1-	1	1-
p-Ethyltoluene	9	L	0	1-	0	0	0	0	0
p-Cresol	15	H	1	1	1	1	1	1-	1-
m-Cresol	15	L	0	1-	0	0	0	0	0

[a]Interpretation by an experienced person.

[b]RTI Mass Spectral Search System.

[c]Fourier Transformed Mass Spectral Search.

[d]Mass spectral search software on Incos Data System (Finnigan Corp.).

[e]No Reindfleisch deconvolution pretreatment.

[f]Reindfleisch deconvolution pretreatment of data prior to search.

[g]M = medium, L = low, H = high.

Table A3. CHEMICALS IDENTIFIED IN MIXTURE NO. 3

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	L[g]	0	0	0	0	0	0	0
Acetonitrile	7	H	0	0	0	0	0	0	0
2-Methylfuran	5	L	1	1-	1-	1-	5-	1	1
Ethyl acetate	4	H	1	1	1	1	1	1	1
Pyrrolidine	8	L	0	0	0	0	0	0	0
2-Pentanone	6	H	1	3	1	3	3	1	1
3-Pentanone	6	L	1	1	1	1	1	1	1
Ethyl acrylate	4	H	1	1	1	1	1	1	1
n-Propyl acetate	4	L	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	H	1	1	1	1	1	1	1
m-Xylene	9	L	1	1	1	1	1-	1-	1-
p-Xylene	9	H	0	0	0	0	0	0	0
Di-n-butyl ether	5	L	0	0	0	0	0	0	0
n-Butyl acrylate	4	H	1	1	1	1	1	1	1
m-Ethyltoluene	9	L	1	1-	2-	1	1	0	2-
p-Ethyltoluene	9	H	1	1	2-	1-	0	1-	1
p-Cresol	15	L	1	1-	1-	1	1	1-	1-
m-Cresol	15	H	1	0	5-	0	0	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A4. CHEMICALS IDENTIFIED IN MIXTURE NO. 4

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Propionaldehyde	3	M[g]	0	0	0	0	0	0	2
Acetone	6	M	1	3	1	3	5	1	0
Methylene chloride	10	M	1	1	1	0	1	1	1
t-Butanol	1	M	0	1	1	1	1	1	1
2-Methylfuran	5	M	1	0	1-	1-	1-	1	1
Perfluorobenzene	11	M	1	1	1	1	1	1	1
Perfluorotoluene	11	M	1	0	1	1	1	1	1
1,2-Dichloroethane	10	H	0	1	1	1	1	1	1
Benzene	9	H	1	1	1	1	1	1	1
Thiophene	13	M	1	1	1	4	0	1	1
2-Pentanone	6	M	1	4	2	2	2	1	1
Acetic acid	14	M	0	0	0	0	0	0	0
Methyl methyacrylate	4	M	1	1	2	0	0	1	1
n-Heptane	1	M	0	2	1	0	3-	1	1
Piperidine	8	M	0	0	0	0	0	0	0
Pyridine	8	M	1	1	1	1	1	1	1
Toluene	9	M	1	1	1	1	1	1	1
2-Methylthiophene	13	M	1	1	1	0	1	1	1-
Butyl acetate	4	M	1	1	1	0	1	1	1
n-Octane	1	M	0	1	1	0	0	1	1-
Styrene	9	M	1	1	1	1	1	1	1
Heptaldehyde	3	M	0	1	1	1	1-	1	1

(continued)

Table A4 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
m-Ethyltoluene	9	M	1	1-	1-	1	1	1	1-
Benzonitrile	7	M	1	1	1	1	1	1	1
1,3,5-Trimethylbenzene	9	M	1	1	1-	1-	0	1	0
Butyl methacrylate	4	M	1	2	2	0	0	1	1
p-Dichlorobenzene	11	M	1	1-	1-	1-	1-	1	1
n-Decane	1	M	1	0	1	0	0	1	1
Nitrobenzene	8	M	1	1	1	1	1	1	1
p-Tolualdehyde	3	M	0	0	3	0	1	1	1
2-Methylbenzofuran	5	M	1	1	1	1	1	1	1
n-Undecane	1	M	1	1	1-	0	0	1	1
Naphthalene	9	M	1	1	3	2	1	1	1
1-Benzothiophene	13	M	1	1	1	1	1	1	1
n-Dodecane	1	M	1	1	1-	0	0	1	1
2-Benzothiazole	13	M	1	2	2	0	1	1	1
Hexachloro-1,3-butadiene	10	M	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	M	0	0	0	0	0	2	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A5. CHEMICALS IDENTIFIED IN MIXTURE NO. 5

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Propionaldehyde	3	H[g]	0	5	2	1	1	1	1
Acetone	6	L	0	0	0	0	0	1	0
Methylene chloride	10	H	1	1	1	1	0	1	1
t-Butanol	2	L	0	0	3	0	1	1	1
2-Methylfuran	5	L	1	0	0	0	1-	1	0
Perfluorobenzene	11	H	1	1	1	1	1	1	1
Perfluorotoluene	11	H	1	0	1	1	1	1	1
1,2-Dichloroethane	10	L	0	0	1	0	1	1	1
Benzene	9	L	1	1	1	1	2	1	1
Thiophene	13	H	1	1	1	5	0	1	1
2-Pentanone	6	H	1	3	4	3	3	1	1
Acetic Acid	14	L	0	0	0	0	0	0	0
Methyl methyacrylate	4	H	1	1	1	0	0	1	1
n-Heptane	1	L	0	0	0	0	0	0	2
Piperidine	8	H	0	0	0	0	0	0	0
Pyridine	8	L	0	0	0	0	0	1	0
Toluene	9	L	1	1	1	1	2	1	1
2-Methylthiophene	13	H	1	1	1-	1	1	1	1
Butyl acetate	4	H	1	1	1	1	1	1	1
n-Octane	1	L	0	1	1-	0	0	5	0
Styrene	9	H	1	1	1	1	1	1	1

(continued)

Table A5 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Heptaldehyde	3	L	0	1	1	1	1-	0	1
m-Ethyltoluene	9	H	1	1	2-	1-	1-	1	0
Benzonitrile	7	L	1	0	1	1	1	1	0
1,3,5-Trimethylbenzene	9	H	1	1	1-	1-	1-	1	1
Butyl methacrylate	4	L	0	2	2	0	0	1	1
p-Dichlorobenzene	11	H	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1-	1	0	0	1	1
Nitrobenzene	8	L	0	0	0	0	0	1	0
p-Tolualdehyde	12	H	1	1	1	1	1-	1	1
2-Methylbenzofuran	5	H	1	1	1	1	1-	1	1
n-Undecane	1	L	1	1	1	0	0	1	1
Naphthalene	9	H	1	2	2	0	2	1	1
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	H	1	1	1	0	0	1	1
2-Benzothiazole	13	L	1	0	0	2	2	1	1
Hexachloro-1,3-butadiene	10	L	1	1	1	0	1	1	1
o-Chloronitrobenzene	11	H	1	1	1	0	1	1	1

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fouirer Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A6. CHEMICALS IDENTIFIED IN MIXTURE NO. 6

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Propionaldehyde	3	L[g]	0	0	0	0	0	0	0
Acetone	6	H	1	3	1	5	5	1	1
Methylene chloride	10	L	1	1	1	1	0	1	1
t-Butanol	2	H	0	1	1	1	3	1	1
2-Methylfuran	5	H	1	1-	1-	1-	1-	1	1
Perfluorobenzene	11	L	0	0	1	0	1	1	1
Perfluorotoluene	11	L	0	0	1	0	0	1	1
1,2-Dichloroethane	10	H	1	1	1	1	1	1	1
Benzene	9	H	1	1	1	1	1	1	1
Thiophene	13	L	1	1	2	3	0	1	1
2-Pentanone	6	L	1	2	1	1	2	1	1
Acetic acid	14	H	0	0	0	0	0	0	0
Methyl methyacrylate	4	L	0	0	0	0	0	0	0
n-Heptane	1	H	1	1	1	0	3-	1	1
Piperidine	8	L	0	0	0	0	0	0	0
Pyridine	8	M	1	1	1	0	0	1	1
Toluene	9	H	1	1	1	1	1	1	1
2-Methylthiophene	13	L	1	0	1-	1-	1	1	1
Butyl acetate	4	L	0	0	1	1	1	0	1
n-Octane	1	M	1	1	1	0	3-	1	1
Styrene	9	L	1	1	1	1	1	1	1

(continued)

Table A6 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Heptaldehyde	3	H	1	1	1	1-	1-	1	1
m-Ethyltoluene	9	L	0	0	1-	1-	1-	1-	1-
Benzonitrile	7	H	1	1	1	1	1	1	1
1,3,5-Trimethylbenzene	9	L	1	1-	1-	1-	1-	1	1
Butyl methacrylate	4	H	1	2	2	0	0	1	1
p-Dichlorobenzene	11	L	1	1-	1-	1-	1-	1	1-
n-Decane	1	H	1	1	1	0	0	1	1
Nitrobenzene	8	H	1	1	1	1	1	1	1
p-Tolualdehyde	12	L	0	0	0	0	0	0	0
2-Methylbenzofuran	13	L	1	1	1	1	1	1	1
n-Undecane	1	H	1	1-	1-	0	0	1	1
Naphthalene	9	L	1	2	2	1	1	1	2
1-Benzothiophene	13	H	1	1	1	1	1	1	1
n-Dodecane	1	L	0	0	0	0	0	1	0
2-Benzothiazole	13	H	1	2	2	1	1	1	1
Hexachloro-1,3-butadiene	10	H	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	L	0	0	0	0	0	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A7. CHEMICALS IDENTIFIED IN MIXTURE NO. 7

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acetonitrile	7	M[g]	0	0	0	0	0	0	0
Propionaldehyde	3	M	0	0	0	0	0	0	0
Acetone	6	M	1	0	1	0	1	1	1
Vinylidene chloride	10	M	1	1-	1-	1-	1-	1	1
Methylene chloride	10	M	1	1	1	3	0	1	1
t-Butanol	2	M	0	1	1	1	0	1	1
2-Methylfuran	5	M	1	1-	2-	1-	1-	1	1
Perfluorobenzene	11	M	1	1	1	1	1	1	1
n-Hexane	1	M	1	4	4	0	0	0	0
Perfluorotoluene	11	M	1	1	1	1	1	1	1
1,2-Dichloroethane	10	H	1	1	1	1	1	1	1
1,1,1-Trichloroethane	10	M	1	0	1	1	1	1	1
Benzene	9	H	1	1	1	1	1	1	1
Thiophene	13	M	1	1	1	5	0	1	1
2-Pentanone	6	M	1	1	1	2	3	0	0
Acetic acid	14	M	0	0	0	0	0	0	0
1,2-Dichloropropane	10	M	1	1-	1-	1	1	1	1
Methyl methacrylate	4	M	0	0	0	0	0	0	0
n-Heptane	1	M	1	1	1	0	0	1	1
n-Propyl acetate	14	M	1	1	1	1	1	0	1

(continued)

Table A7 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Piperidine	8	M	0	0	0	0	0	0	0
Pyridine	8	M	1	1	1	1	1	1	2
Toluene	9	M	1	1	1	1	1	1	1
2-Methylthiophene	13	M	1	1	1-	1	1	0	1
n-Butyl acetate	4	M	1	1	1	1	1	1	1
n-Octane	1	M	0	1	1	0	0	1	2
Tetrachloroethylene	10	M	1	1	1	1	1	1	1
Styrene	9	M	1	1	1	1	1	0	1
n-Heptaldehyde	3	M	0	1	0	0	0	1	0
o-Xylene	9	M	1	1-	1-	1-	1-	1	1-
m-Ethyltoluene	9	M	1	1-	4-	2-	0	1-	1
Benzonitrile	7	M	1	1	0	1	0	1	0
p-Ethyltoluene	9	M	1	1-	4-	2-	0	0	0
1,3,5-Trimethylbenzene	9	M	0	1-	2-	1-	1-	1	1
Butyl methacrylate	4	M	1	2	1	0	0	1	1
Phenol	15	M	1	1	1	1	1	1	1
p-Dichlorobenzene	11	M	1	1-	1-	1-	1-	1	1
n-Decane	1	M	1	1	1	0	0	1	1
m-Cresol	15	M	1	1	1-	1-	1-	1	1
Nitrobenzene	8	M	1	1	1	1	1	0	1
p-Tolualdehyde	12	M	0	0	2	0	1	1	0

(continued)

Table A7 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
2-Methylbenzofuran	5	M	1	1	1	1	1	1	1
n-Undecane	1	M	1	2	1-	0	0	1	2
Naphthalene	9	M	1	1	2	2	1	1	1
1-Benzothiophene	13	M	1	1	1	1	1	1	1
n-Dodecane	1	M	1	1	1	0	0	1	1
2-Benzothiazole	13	M	1	0	0	1	0	1	0
Hexachloro-1,3-butadiene	10	M	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	M	1	0	0	0	0	0	0
Quinoline	8	M	0	0	0	0	0	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A8. CHEMICALS IDENTIFIED IN MIXTURE NO. 8

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acetonitrile	7	L[g]	0	0	0	0	0	0	0
Propionaldehyde	3	H	0	0	0	0	0	0	2
Acetone	6	L	1	3	0	0	0	1	0
Vinylidene chloride	10	L	1	1	1-	1-	1-	1	1-
Methylene chloride	10	H	1	1	1	1	1	1	1
t-Butanol	2	L	0	1	1	1	1	1	1
2-Methylfuran	5	L	1	1-	1-	1-	1-	1	1
Perfluorobenzene	11	H	1	0	0	0	0	1	0
n-Hexane	1	L	1	1	1	1	1	1	1
Perfluorotoluene	11	H	1	1	1	0	0	1	1
1,2-Dichloroethane	10	L	1	1	1	1	1	1	1
1,1,1-Trichloroethane	10	L	1	2	1	2	1	1	1
Benzene	9	L	1	1	2	1	1	1	1
Thiophene	13	H	1	1	1	2	4	1	1
2-Pentanone	6	H	1	3	1	2	3	1	1
Acetic acid	14	L	0	0	0	0	0	1	1
1,2-Dichloropropane	10	L	1	1-	1	1	1	1	1
Methyl methacrylate	4	H	0	0	0	0	0	0	0
n-Heptane	1	L	1	1	1	0	0	1	1
n-Propyl acetate	14	L	0	1	1	1	1	1	1

(continued)

Table A6 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Piperidine	8	H	0	0	0	0	0	0	0
Pyridine	8	L	1	1	4	1	0	1	1
Toluene	9	L	1	1	1	1	1	1	1
2-Methylthiophene	13	H	1	1	1-	1-	1	1	1
n-Butyl acetate	4	H	1	1	1	1	1	1	1
n-Octane	1	L	1	1	1	0	0	1	1
Tetrachloroethylene	10	L	1	1	1	1	1	1	1
Styrene	9	H	1	1	1	1	1	1	1
n-Heptaldehyde	3	L	0	1	1	1	5	0	1
o-Xylene	9	L	1	1-	1-	1-	1-	1	1
m-Ethyltoluene	9	H	1	1-	0	3	2-	1	1
Benzonitrile	7	L	1	1	1	1	1	1	1
p-Ethyltoluene	9	L	0	0	0	0	0	1	1
1,3,5-Trimethylbenzene	9	H	1	1-	1-	1-	1-	1	1
n-Butyl methacrylate	4	L	1	-	2	0	0	2	1
Phenol	15	L	1	1	1	1	0	1	1
p-Dichlorobenzene	11	H	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1	1	0	0	1	1
m-Cresol	15	L	1	0	0	1-	0	0	1-
Nitrobenzene	8	L	1	1	1	1	1	1	1
p-Tolualdehyde	12	H	0	0	0	0	0	1	1

(continued)

Table A8 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
2-Methylbenzofuran	5	H	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	2	0	0	1	1
Naphthalene	9	H	1	1	1	2	1	1	1
1-Benzothiophene	13	L	1	1	1-	1	1	1	1
n-Dodecane	1	H	0	0	0	0	0	0	0
2-Benzothiazole	13	L	1	2	2	1	0	1	1
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	H	0	0	0	0	0	1	1
Quinoline	8	L	0	0	0	0	0	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A9. CHEMICALS IDENTIFIED IN MIXTURE NO. 9

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
Acetonitrile	7	H[g]	0	0	0	0	0	0	
Propionaldehyde	3	L	0	0	0	0	0	0	
Acetone	6	L	0	0	0	0	0	0	
Vinylidene chloride	10	H	1	1-	1	1-	1-	1	
Methylene chloride	10	L	1	1	1	0	0	1	
t-Butanol	2	L	1	0	1	0	0	0	
2-Methylfuran	5	L	1	1-	1-	1-	1-	1	
Perfluorobenzene	11	L	0	0	0	0	0	1	
n-Hexane	1	H	1	1	1	5	1	1	
Perfluorotoluene	11	L	1	0	1	0	0	1	
1,2-Dichloroethane	10	L	1	1	1	1	1	1	
1,1,1-Trichloroethane	10	H	1	1	1	1	1	1	
Benzene	9	H	1	1	1	1	1	0	
Thiophene	13	L	1	1	1	4	0	1	
2-Pentanone	6	L	1	4	1	3	2	1	
Acetic acid	14	L	0	0	0	0	0	1	
1,2-Dichloropropane	10	H	1	1-	1-	1	0	1	
Methyl methacrylate	4	L	1	2	0	0	0	1	
n-Heptane	1	L	1	2	1	0	0	0	
n-Propyl acetate	4	H	1	1	1	1	1	1	
Piperdine	8	L	0	0	0	0	0	0	

(continued)

Table A9 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
Pyridine	8	H	0	0	0	0	0	1	
Toluene	9	H	1	1	1	1	1	1	
2-Methylthiophene	13	L	1	1	1	1-	1	1	
n-Butyl acetate	4	L	0	2	1	1	1	1	
n-Octane	1	L	0	0	0	0	0	0	
Tetrachloroethylene	10	H	1	1	1	1	1	1	
Styrene	9	L	1	1	1	1	1	1	
n-Heptaldehyde	3	L	0	0	0	0	0	0	
o-Xylene	9	H	1	1-	1-	1-	1	1-	
m-Ethyltoluene	9	L	1	1-	1	2	1	1	
Benzonitrile	7	L	0	0	1	0	1	1	
p-Ethyltoluene	9	H	1	3-	1	0	1	0	
1,3,5-Trimethylbenzene	9	L	1	1-	0	0	0	1	
n-Butyl methacrylate	4	L	0	1	2	0	0	0	
Phenol	15	H	1	1	5	1	1	1	
p-Dichlorobenzene	11	L	1	1-	1-	1-	1-	1	
n-Decane	1	H	1	1	0	0	0	1	
m-Cresol	15	H	1	1	1	1-	1-	1	
Nitrobenzene	8	L	1	0	4	0	0	1	
p-Tolualdehyde	12	L	1	0	2	0	2-	1	
2-Methylbenzofuran	5	L	1	1	1	1	1	1	
n-Undecane	1	H	1	1	1	0	0	1	

(continued)

Table A9 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
Naphthalene	9	L	1	1	1	1	2	1	
1-Benzothiophene	13	H	1	1	1	1	1	1	
n-Dodecane	1	L	1	1	1	0	0	1	
2-Benzothiazole	13	H	1	0	2	1	0	1	
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	
o-Chloronitrobenzene	11	L	0	0	1-	0	1-	1	
Quinoline	8	H	1	1	1-	0	2	1	

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

[h] Data failed to pass through deconvolution.

Table A10. CHEMICALS IDENTIFIED IN MIXTURE NO. 10

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	M[g]	0	0	0	0	0	0	0
Acetonitrile	7	M	0	0	0	0	0	0	0
Propionaldehyde	3	M	0	0	0	0	0	0	0
Acetone	6	M	1	0	0	0	0	1	0
Acrylonitrile	7	M	0	0	0	0	0	0	1-
Vinylidene chloride	10	M	1	1-	1-	1-	1-	1	1
Methylene chloride	10	M	1	1	1	0	0	1	1
t-Butanol	2	M	1	4	1	5	0	1	1
2-Methylfuran	5	M	1	2-	1-	1-	1-	1	1
Perfluorobenzene	11	M	1	1	1	1	1	1	1
n-Hexane	1	M	0	3	4	0	0	1	1
Ethyl acetate	4	M	1	1	1	1	1	1	1
Perfluorotoluene	11	M	1	1	1	0	1	1	1
1,2-Dichloroethane	10	H	1	1	1	1	1	1	1
1,1,1-Trichloroethane	10	M	1	1	1	1	1	1	1
Benzene	9	H	1	1	1	1	1	1	1
Thiophene	13	M	1	1	1	5	0	1	1
Pyrrolidine	8	M	0	0	0	0	0	0	1-
2-Pentanone	6	M	1	5	1	3	3	1	1
Acetic acid	14	M	0	0	0	0	0	1	0
1,2-Dichloropropane	10	M	1	4-	1	1	1	1	1

(continued)

Table A10 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Methyl methacrylate	4	M	1	0	2	0	0	1	1-
n-Heptane	1	M	1	1	1	0	0	1	1
n-Propyl acetate	4	M	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	M	0	0	0	0	0	1	0
Piperidine	8	M	0	0	0	0	0	0	0
Pyridine	8	M	1	1	1	1	1	1	1
Toluene	9	M	1	1	1	1	1	1	1
2-Methylthiophene	13	M	1	1	1-	1	1	1-	1-
Butyl acetate	4	M	0	1	1	1	1	0	1
n-Octane	1	M	0	2	1	0	1	1	4
Tetrachloroethylene	10	M	1	1	1	1	1	1	1
n-Butyl acrylate	4	M	1	1	1	0	1	0	0
Styrene	9	M	1	1	1	1	1	1	1
n-Heptaldehyde	3	M	0	1	1	0	0	0	3
o-Xylene	9	M	1	1-	1-	1-	1-	1-	1
m-Ethyltoluene	9	M	1	1-	3	1	2	0	0
Benzonitrile	7	M	1	0	1	0	1	1	1
p-Ethyltoluene	9	M	1	1-	3-	0	0	1	1
1,3,5-Trimethylbenzene	9	M	0	1-	1-	1-	1-	1	1
Butyl methacrylate	4	M	1	1	2	0	0	1	1
Phenol	15	M	1	1	2	0	0	1	1

(continued)

Table A10 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
p-Dichlorobenzene	11	M	1	1-	1-	1-	1-	1	1
n-Decane	1	M	1	1	1	0	0	1	1
p-Cresol	15	M	1	1	1	1	1	0	1-
m-Cresol	15	M	0	0	0	1-	0	1	1
Nitrobenzene	8	M	1	0	0	0	0	1	0
p-Tolualdehyde	12	M	0	0	1-	0	0	1	1
2-Methylbenzofuran	5	M	1	1	1	1	1	1	0
n-Undecane	1	M	1	1	1	0	0	1	1
Naphthalene	9	M	1	1	1	1	1	1	1
1-Benzothiophene	13	M	1	1	1	1	1	1	1
n-Dodecane	1	M	1	1	1	0	0	3	1
2-Benzothiazole	13	M	1	0	0	1	1	1	0
Hexachloro-1,3-butadiene	10	M	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	M	0	0	0	0	0	0	0
Quinoline	8	M	0	0	0	0	0	2	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A11. CHEMICALS IDENTIFIED IN MIXTURE NO. 11

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	H[g]	0	0	1	0	1	0	1
Acetonitrile	7	L	0	0	1-	0	1-	0	0
Propionaldehyde	3	L	0	0	0	0	0	0	0
Acetone	6	L	1	0	0	4	0	1	1
Acrylonitrile	7	H	1	1	1	1	1	1	1
Vinylidene chloride	10	L	1	0	0	0	0	1	0
Methylene chloride	10	L	1	1	1	1	0	1	1
t-Butanol	2	L	1	0	1	1	2	1	1
2-Methylfuran	5	L	1	1-	1-	0	2-	1	2
Perfluorobenzene	11	L	1	0	0	0	0	0	0
n-Hexane	1	L	1	1	1-	1	1	1	1
Ethyl acetate	4	H	1	1	1-	0	1	1	1
Perfluorotoluene	11	L	1	2	1	1	1	1	1
1,2-Dichloroethane	10	L	1	1	1	1	1	0	1
1,1,1-Trichloroethane	10	L	1	2	1	1	1	1	1
Benzene	9	L	1	2	1	1	1	1	1
Thiophene	13	L	1	1	1	5	0	1	1
Pyrrolidine	8	H	0	0	0	0	0	0	0
2-Pentanone	6	L	1	3	1	3	2	1	1
Acetic acid	14	L	0	0	0	0	0	0	0
1,2-Dichloropropane	10	L	1	1	0	1	1	1	1
Methyl methacrylate	4	L	0	1	2	0	0	0	1

(continued)

Table A11 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
n-Heptane	1	L	0	1	2-	1	0	1	0
n-Propyl acetate	4	L	0	1	1	0	0	1	1
α-Methylbutyronitrile	7	H	0	1	1	1	1	1	1
Piperidine	8	L	0	0	0	0	0	0	0
Pyridine	8	L	0	0	0	0	0	0	0
Toluene	9	L	1	1	1	1	1	1	1
2-Methylthiophene	13	L	1	1-	1-	1	1	1-	1
n-Butyl acetate	4	L	1	1	1	1	1	1	1
n-Octane	1	L	0	2	1	0	0	0	1
Tetrachloroethylene	10	L	1	1	1	1	1	0	1
n-Butyl acrylate	4	H	1	1	1	1	1	1	1
Styrene	9	L	1	1	1	1	1	1	1
n-Heptaldehyde	3	L	0	0	0	0	0	0	1
o-Xylene	9	L	1	0	1-	0	0	1-	0
m-Ethyltoluene	9	L	1	4	3	3	2	1	0
Benzonitrile	7	L	1	1	1	4	1	5	1
p-Ethyltoluene	9	L	1	2	2	0	0	0	0
1,3,5-Trimethylbenzene	9	L	0	1-	1-	0	1-	1	1-
Butyl methacrylate	4	L	1	2-	0	0	0	1	1
Phenol	15	L	1	1	0	0	0	1	0
p-Dichlorobenzene	11	L	1	1-	1-	0	1-	1	1

(continued)

Table A11 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
n-Decane	1	L	1	1	1	0	0	1	1
p-Cresol	15	H	1	1	1	1-	0	0	0
m-Cresol	15	L	0	0	0	0	0	1	1
Nitrobenzene	8	L	1	1	1	1	1	1	3
p-Tolualdehyde	12	L	1	0	0	0	0	1	0
2-Methylbenzofuran	5	L	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	1	0	0	1	0
Naphthalene	9	L	1	2	1	1	1	0	1
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	L	1	1	1	0	0	1	1
2-Benzothiazole	13	L	1	0	2	1	2	2	3
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	0
o-Chloronitrobenzene	11	L	1	0	1-	0	1-	1	1
Quinoline	8	L	0	0	0	0	0	3	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A12. CHEMICALS IDENTIFIED IN MIXTURE NO. 12

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	L[g]	0	0	0	0	0	0	1
Acetonitrile	7	L	0	0	0	0	0	0	0
Propionaldehyde	3	HS	0	3	3	1	1	1	1
Acetone	6	L	0	0	0	0	0	0	0
Acrylonitrile	7	L	0	1	1	0	0	0	0
Vinylidene chloride	10	L	1	1-	1-	1-	1-	1	1
Methylene chloride	10	HS	1	1	1	1	1	1	1
t-Butanol	2	L	0	1	1	0	0	1	1
2-Methylfuran	5	L	0	1-	1-	0	0	1	1
Perfluorobenzene	11	HS	1	1	1	1	1	1	1
n-Hexane	1	L	0	0	0	0	0	0	0
Ethyl acetate	4	L	0	1	1	1	1	1	1
Perfluorotoluene	11	HS	1	1	1	1	1	1	1
1,2-Dichloroethane	10	L	0	4	1	0	0	1	1
1,1,1-Trichloroethane	10	L	0	0	0	0	0	1	0
Benzene	9	L	1	1	1	0	2	1	1
Thiophene	13	HS	1	1	1	1	1	1	1
Pyrrolidine	8	L	0	0	0	0	0	0	0
2-Pentanone	6	HS	1	0	0	0	3	1	1
Acetic acid	14	L	1	0	0	0	0	0	0
1,2-Dichloropropane	10	L	1	1-	1-	1	1	1	1

(continued)

Table A12 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Methyl methacrylate	4	HS	0	1	1	0	5	1	1
n-Heptane	1	L	0	0	0	0	0	0	0
n-Propyl acetate	4	L	1	1	1	0	0	1	1
α-Methylbutyronitrile	7	L	0	2	2	0	0	0	1
Piperidine	8	HS	0	0	0	0	0	0	0
Pyridine	8	L	1	1	1	1	1	1	1
Toluene	9	L	0	0	0	0	0	1	1
2-Methylthiophene	13	HS	1	0	0	0	1	1	0
Butyl acetate	4	HS	1	1	1	1	1	0	2
n-Octane	1	L	1	0	0	0	0	2	1-
Tetrachloroethylene	10	L	0	1	1	0	0	0	1
n-Butyl acrylate	4	L	0	1	1	0	0	1	1
Styrene	9	HS	1	0	0	1	1	1	1
n-Heptaldehyde	3	L	0	0	2-	0	0	0	0
o-Xylene	9	L	1	1-	1-	1-	1-	1	1
m-Ethyltoluene	9	HS	1	0	0	0	0	1	0
Benzonitrile	7	L	0	1	1	4	0	1	0
p-Ethyltoluene	9	L	0	0	0	1	1	0	1
1,3,5-Trimethylbenzene	9	HS	1	0	0	1-	1-	1-	0
Butyl methacrylate	4	L	1	3	3	0	0	3	1
Phenol	15	L	1	1	0	1	1	1	0

(continued)

Table A12 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
p-Dichlorobenzene	11	HS	1	0	0	1-	1-	0	0
n-Decane	1	L	0	0	0	0	0	1	0
p-Cresol	15	L	1	1-	1-	1	1	1	1-
m-Cresol	15	L	0	0	0	0	1-	1	0
Nitrobenzene	8	L	0	0	0	0	0	1	0
p-Tolualdehyde	12	HS	1	0	0	1	1	1	0
2-Methylbenzofuran	5	HS	1	3	0	1	1	1	2
n-Undecane	1	L	0	0	0	0	0	1	0
Naphthalene	9	HS	1	5	5	2	2	2	0
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	HS	1	0	0	0	0	1	0
2-Benzothiazole	13	L	0	2	2	3	0	4	1-
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	HS	1	0	0	1-	1-	1	1
Quinoline	8	L	0	0	0	2	2	0	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high, HS = highly saturated.

Table A13. CHEMICALS IDENTIFIED IN MIXTURE NO. 13

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	M[g]	0	0	0	0	3	0	0
Acetonitrile	7	M	0	0	0	0	0	0	0
Propionaldehyde	3	M	0	0	1	0	1	2	0
Acetone	6	M	1	0	0	0	0	0	0
Ethanol	2	M	0	0	5	0	1	1	1
Acrylonitrile	7	M	1	0	1	0	1	0	1
Vinylidene chloride	10	M	1	1-	1-	1-	1-	1	1
Methylene chloride	10	M	1	1	1	4	1	1	1
t-Butanol	2	M	1	1	1	1	1	1	1
2-Methylfuran	5	M	1	2-	1-	1-	1-	1	1
Perfluorobenzene	11	M	1	1	1	1	1	1	1
n-Hexane	1	M	1	4	0	0	0	0	0
Ethyl acetate	4	M	1	0	0	0	0	1	0
Chloroform	10	M	1	1	1	2	0	1	1
Perfluorotoluene	11	M	1	1	1	0	1	1	1
1,2-Dichloroethane	10	H	1	1	1	1	1	1	1
1,1,1-Trichloroethane	10	M	1	2	1	1	1	1	1
Benzene	9	H	1	1	4	1	1	1	1
Thiophene	13	M	1	1	1	0	1	1	1
Pyrrolidine	8	M	0	0	0	3	0	0	0
2-pentanone	6	M	1	2	1	1	2	1	1
Acetic acid	14	M	0	0	0	0	0	0	0

(continued)

Table A13 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
1,2-Dichloropropane	10	M	1	1	1	1	1	1	1
3-Pentanone	6	M	0	1	1	1	1	1	1
Methyl methacrylate	4	M	1	1	2	3	0	1	1
n-Heptane	1	M	1	1	1	0	0	1	1
n-Propyl acetate	4	M	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	M	0	0	1	4	1	1	1
Piperidine	8	M	0	0	0	0	0	0	0
Pyridine	8	M	1	1	1	1	1	1	1
Toluene	9	M	1	1	1	1	1	1	1
2-Methylthiophene	13	M	1	1	1-	1	1	1	1-
n-Butyl acetate	4	M	1	1	1	1	1	1	1
n-Octane	1	M	1	1	1	1-	0	1	1
Tetrachloroethylene	10	M	1	1	1	1	1	1	1
Di-n-butyl ether	5	M	0	1	1	2	3	1	0
n-Butyl acrylate	4	M	1	0	0	0	0	1	0
Styrene	9	M	1	1	1	1	1	1	1
n-Heptaldehyde	3	M	0	1	1	1-	0	0	1
o-Xylene	9	M	1	1-	1-	1-	1-	1	1
m-Ethyltoluene	9	M	1	1-	1	2	1	0	0
Benzonitrile	7	M	1	1	1	0	1	1	0
p-Ethyltoluene	9	M	1	3-	1-	2-	1-	1	5
1,3,5-Trimethylbenzene	9	M	1	1-	0	1-	0	1	1

(continued)

Table A13 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Butyl methacrylate	4	M	1	2	4	0	0	1	1
Phenol	15	M	1	1	1	1	1	1	1
p-Dichlorobenzene	11	M	1	1-	1-	1-	1-	1	1
n-Decane	1	M	1	1	1	0	0	1	1
p-Cresol	15	M	1	1-	1-	1-	1-	0	0
m-Cresol	15	M	0	1-	0	1	0	1	1
Nitrobenzene	8	M	1	1	1	1	3	1	1
p-Tolualdehyde	12	M	1	0	1	0	1-	3	0
2-Methylbenzofuran	13	M	1	1	1	1	1	1	1
n-Undecane	1	M	1	2	2	0	0	1	1
Naphthalene	9	M	1	1	2	2	2	1	2
1-Benzothiophene	13	M	1	1	1	1	1	1	1
n-Dodecane	1	M	1	1	1	0	0	1	1
2-Benzothiazole	13	M	1	0	0	1	3	1	0
Hexachloro-1,3-butadiene	10	M	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	M	0	0	1-	0	0	1	1
Quinoline	8	M	1	2	3	3	3	1	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A14. CHEMICALS IDENTIFIED IN MIXTURE NO. 14

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	H[g]	0	0	1	0	1	1	1
Acetonitrile	7	L	0	0	0	0	0	0	0
Propionaldehyde	3	L	0	0	0	0	0	0	0
Acetone	6	L	0	0	3	0	0	0	1
Ethanol	2	L	0	0	0	0	0	5	0
Acrylonitrile	7	H	1	1	0	1	1	1	0
Vinylidene chloride	10	L	1	1	1	0	0	1	0
Methylene chloride	10	L	1	1	1	1	4	1	1
t-Butanol	2	L	1	0	1	0	4	1	
2-Methylfuran	5	L	1	1-	1	1-	1-	1	1
Perfluorobenzene	11	L	1	0	0	0	0	0	0
n-Hexane	1	L	0	0	1	0	5	1	1
Ethyl acetate	4	H	1	1	1	1	1	1	1
Chloroform	10	L	1	0	0	0	0	1	1
Perfluorotoluene	11	L	1	0	0	0	0	1	1
1,2-Dichloroethane	10	L	1	1	1	1	1	1	4
1,1,1-Trichloroethane	10	L	1	2	1	1	1	1	1
Benzene	9	L	1	1	4	1	3	1	1
Thiophene	13	L	1	1	1	5	4	1	1
Pyrrolidine	8	H	0	0	0	5	0	0	0
2-pentanone	6	L	1	0	2	3	2	1	1
Acetic acid	14	L	1	1	1	1	1	1	1

(continued)

Table A14 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
1,2-Dichloropropane	10	L	1	1	2-	1	1	1	1
3-Pentanone	6	L	1	1	1	1	1	1	1
Methyl methacrylate	4	L	1	1	2	0	0	1	0
n-Heptane	1	L	1	1	1	1	0	1	1
n-Propyl acetate	4	L	1	1	1	1	0	1	1
α-Methylbutyronitrile	7	H	0	1	1	1	3	1	1
Piperidine	8	L	0	1	0	0	0	0	0
Pyridine	8	L	0	0	0	0	0	1	0
Toluene	9	L	1	1	1	1	1	1	1
2-Methylthiophene	13	L	1	1	1-	1	1	1-	1
n-Butyl acetate	4	L	1	1	1	1	1	1	1
n-Octane	1	L	1	1	1	0	0	1	1
Tetrachloroethylene	10	L	1	1	1	1	1	1	1
Di-n-butyl ether	5	L	0	1	1	2	3	3	0
n-Butyl acrylate	4	H	1	1	1	1	1	1	0
Styrene	9	L	1	1	1	1	1	1	0
n-Heptaldehyde	3	L	0	0	0	0	0	0	0
o-Xylene	9	L	1	0	0	0	1-	1	1
m-Ethyltoluene	9	L	1	1-	0	0	0	1	3-
Benzonitrile	7	L	1	1	1	1	1	1	1
p-Ethyltoluene	9	L	0	1	0	0	0	0	0
1,3,5-Trimethylbenzene	9	L	1	1-	1-	1-	1-	1	1

(continued)

Table A14 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Butyl methacrylate	4	L	1	2	2	0	0	1	1
Phenol	15	L	1	1	0	2	0	1	0
p-Dichlorobenzene	11	L	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1	1	0	0	1	1
p-Cresol	15	H	1	1	1	1	1	0	1
m-Cresol	15	L	0	1-	0	0	0	1	0
Nitrobenzene	8	L	1	1	3	1	2	1	0
p-Tolualdehyde	12	L	1	5-	2-	0	3	1	1
2-Methylbenzofuran	5	L	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	1	0	0	1	1
Naphthalene	9	L	1	1	1	1	2	1	1
1-Benzothiophene	13	L	1	1	1	1	1	1	0
n-Dodecane	1	L	1	1	1	0	0	1	1
2-Benzothiazole	13	L	1	0	0	3	1	1	1
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	L	1	0	1-	0	1-	1	1
Quinoline	8	L	0	0	4	0	0	1	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A15. CHEMICALS IDENTIFIED IN MIXTURE NO. 15

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	L[g]	0	0	0	0	0	0	0
Acetonitrile	7	L	0	0	0	0	0	0	0
Propionaldehyde	3	H	1	0	0	5	0	0	0
Acetone	6	L	0	0	0	0	0	1	0
Ethanol	2	L	0	0	0	0	0	0	0
Acrylonitrile	7	L	0	0	0	0	0	1	0
Vinylidene chloride	10	L	1	2	1-	1-	1-	1	1
Methylene chloride	10	H	1	1	1	1	5	1	1
t-Butanol	2	L	1	0	3	1	5	1	1
2-Methylfuran	5	L	1	0	0	0	1-	1	0
Perfluorobenzene	11	H	1	1	1	1	1	1	1
n-Hexane	1	L	0	0	0	0	0	0	0
Ethyl acetate	4	L	1	1	1	1	1	1	1
Chloroform	10	L	1	0	0	1	1	1	0
Perfluorotoluene	11	H	1	1	1	1	1	1	1
1,2-Dichloroethane	10	L	1	1	0	1	1	1	1
1,1,1-Trichloroethane	10	L	1	0	0	0	0	1	0
Benzene	9	L	1	1	2	1	1	1	1
Thiophene	13	H	1	1	1	5	5	1	1
Pyrrolidine	8	L	0	0	0	0	0	0	0
2-pentanone	6	H	1	3	2	3	2	1	1
Acetic acid	14	L	0	1	0	1	0	0	0

(continued)

Table A15 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
1,2-Dichloropropane	10	L	1	1	1-	1	1	1	0
3-Pentanone	6	L	1	1	1	1	1	1	1
Methyl methacrylate	14	H	1	1	1	0	1	1	1
n-Heptane	1	L	0	0	0	0	0	0	0
n-Propyl acetate	4	L	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	L	0	0	0	0	0	1	0
Piperidine	8	H	0	0	0	0	0	0	0
Pyridine	8	L	1	1	1	1	1	1	1
Toluene	9	L	1	1	1	2	1	1	1
2-Methylthiophene	13	H	1	1	1-	1-	1	1	1
n-Butyl acetate	4	H	1	1	1	1	1	0	1
n-Octane	1	L	1	3	0	0	0	4	0
Tetrachloroethylene	10	L	1	1	1	1	1	1	1
Di-n-butyl ether	5	L	0	0	0	0	0	1	0
n-Butyl acrylate	4	L	1	4	0	0	0	0	0
Styrene	9	H	1	1	1	1	1	1	1
n-Heptaldehyde	3	L	0	1	1	1	1-	0	0
o-Xylene	9	L	1	1-	1-	0	0	0	2-
m-Ethyltoluene	9	H	1	2-	3-	1	0	1	0
Benzonitrile	7	L	1	0	1	0	1	1	1
p-Ethyltoluene	9	L	0	0	3-	0	4-	0	0
1,3,5-Trimethylbenzene	9	H	1	1-	1-	1	1-	1	1

(continued)

Table A15 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Butyl methacrylate	4	L	1	2	2	0	0	1	1
Phenol	15	L	1	1	1	1	1	1	1
p-Dichlorobenzene	11	H	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1	1	0	0	1	1
p-Cresol	15	L	1	1-	1-	1	1	1-	1-
m-Cresol	15	L	0	0	0	0	0	0	0
Nitrobenzene	8	L	0	0	0	0	0	1	0
p-Tolualdehyde	12	H	1	1	1	1	1	1	1
2-Methylbenzofuran	5	H	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	1	0	0	1	1
Naphthalene	9	H	1	2	2	1	2	1	1
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	H	1	1	1	0	0	1	1
2-Benzothiazole	13	L	0	0	2	0	2	1	0
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	H	1	1-	1-	1-	1-	1	1
Quinoline	8	L	0	0	0	0	0	1	0

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

Table A16. CHEMICALS IDENTIFIED IN MIXTURE NO. 16

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
Acrolein	3	M[g]	0	0	0	0	0	0	
Acetonitrile	7	M	0	0	0	0	0	0	
Propionaldehyde	3	M	0	0	0	0	0	0	
Acetone	6	M	1	0	0	0	0	0	
Diethyl ether	5	M	0	0	0	0	0	3	
Ethanol	2	M	0	0	0	0	0	0	
Acrylonitrile	7	M	0	0	0	0	0	0	
Vinylidene chloride	10	M	1	2-	1-	1-	1-	1	
Methylene chloride	10	M	1	1	1	1	1	1	
t-Butanol	2	M	1	1	1	1	1	1	
2-Methylfuran	5	M	1	0	1-	0	1-	1	
Perfluorobenzene	11	M	1	1	1	1	1	1	
n-Hexane	1	M	0	0	1	0	0	2	
Ethyl acetate	4	M	0	1	1	1	1	1	
Chloroform	10	M	1	1	1	1	1	1	
Perfluorotoluene	11	M	1	1	1	0	0	1	
1,2-Dichloroethane	10	H	1	1	1	1	1	1	
1,1,1-Trichloroethane	10	M	1	2	1	1	1	1	
Benzene	9	H	1	1	1	1	1	1	
Thiophene	13	M	1	1	1	1	0	1	
Pyrrolidine	8	M	0	0	0	0	0	0	

(continued)

Table A16 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
2-Pentanone	6	M	1	2	1	3	3	1	
Acetic acid	14	M	0	1	0	1	0	1	
1,2-Dichloropropane	10	M	1	1-	1-	1	1	1	
3-Pentanone	6	M	1	1	1	1	1	1	
Ethyl acrylate	4	M	1	3	1	1	1	1	
Methyl methacrylate	4	M	1	1	1	0	0	1	
n-Heptane	1	M	1	1	1	0	0	1	
n-Propyl acetate	4	M	1	1	1	1	1	1	
α-Methylbutyronitrile	7	M	0	0	3	1	0	1	
Piperidine	8	M	0	0	0	0	0	0	
Pyridine	8	M	1	1	1	1	0	1	
Toluene	9	M	1	1	1	1	1	1	
2-Methylthiophene	13	M	1	1	1-	1	1	1	
n-Butyl acetate	4	M	1	1	1	1	1	1	
n-Octane	1	M	1	1	1	0	0	1	
Tetrachloroethylene	10	M	1	1	1	1	1	1	
Di-n-butyl ether	5	M	0	1	3	2	2	2	
n-Butyl acrylate	4	M	1	1	2	1	1-	1	
Styrene	9	M	1	1	1	1	1	1	
n-Heptaldehyde	3	M	0	0	1	0	0	0	
o-Xylene	9	M	1	1-	1-	1-	1	1-	
1,1,2,2-Tetrachloroethane	9	M	1	1	1	1	1	1	

(continued)

Table A16 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D[h]
m-Ethyltoluene	9	M	1	1-	1	1	2	1-	
Benzonitrile	7	M	1	1	1	1	1	1	
p-Ethyltoluene	9	M	1	1-	3-	2-	2-	0	
1,3,5-Trimethylbenzene	9	M	0	1-	1-	1-	1-	1	
Butyl methacrylate	4	M	1	2	2	0	0	1	
Phenol	15	M	1	1	1	1	2	1	
p-Dichlorobenzene	11	M	1	1-	1-	1-	1-	1	
n-Decane	1	M	1	1	1	0	0	1	
p-Cresol	15	M	1	1	1	1	1	1-	
m-Cresol	15	M	0	1	0	0	0	0	
Nitrobenzene	8	M	1	1	1	1	1	1	
p-Tolualdehyde	12	M	1	0	3	0	0	1-	
2-Methylbenzofuran	5	M	1	1	1	1	1	1	
n-Undecane	1	M	1	1	1	0	0	1	
Naphthalene	9	M	1	1	2	1	1	1	
1-Benzothiophene	13	M	1	1	1	1	1	1	
n-Dodecane	1	M	1	1	1	0	0	1	
2-Benzothiazole	13	M	1	0	0	0	0	2	
Hexachloro-1,3-butadiene	10	M	1	1	1	1	1	1	
o-Chloronitrobenzene	11	M	0	0	0	0	0	1	
Quinoline	8	M	0	0	3	0	3	1	

Footnotes - Table A16

[a]Interpretation by an experienced person.

[b]RTI Mass Spectral Search System.

[c]Fouirer Transformed Mass Spectral Search.

[d]Mass spectral search software on Incos Data System (Finnigan Corp.).

[e]No Reindfleisch deconvolution pretreatment.

[f]Reindfleisch deconvolution pretreatment of data prior to search.

[g]M = medium, L = low, H = high.

[h]Data failed to pass through devonvolution.

Table A17. CHEMICALS IDENTIFIED IN MIXTURE NO. 17

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	L[g]	0	0	0	0	0	0	0
Acetonitrile	7	L	0	0	0	0	0	0	0
Propionaldehyde	3	H	1	0	1	1	1	0	2
Acetone	6	L	0	0	0	0	0	0	0
Diethyl ether	5	L	0	0	0	0	0	0	0
Ethanol	2	L	0	0	0	0	0	0	0
Acrylonitrile	7	L	0	0	0	0	0	0	0
Vinylidene chloride	10	L	1	2	1-	1-	1-	1	1
Methylene chloride	10	H	1	1	1	1	0	1	1
t-Butanol	2	L	1	0	3	1	1	1	1
2-Methylfuran	5	L	1	3-	3-	0	0	1	0
Perfluorobenzene	11	H	1	1	1	1	1	1	1
n-Hexane	1	L	0	0	0	0	0	0	0
Ethyl acetate	4	L	0	1	1	1	1	1	1
Chloroform	10	L	1	3	2	1	0	1	1
Perfluorotoluene	11	H	1	1	1	1	1	0	1
1,2-Dichloroethane	10	L	1	1	1	1	1	1	1
1,1,1-Trichloroethane	10	L	1	3	1	1	2	1	1
Benzene	9	L	1	1	1	1	2	1	1
Thiophene	13	H	1	1	1	5	0	1	1
Pyrrolidine	8	L	0	0	0	0	0	0	0

(continued)

Table A17 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
2-Pentanone	6	H	1	2	1	2	2	1	1
Acetic acid	14	L	1	1	1	1	1	1	1
1,2-Dichloropropane	10	L	1	0	1	1	1	1	1
3-Pentanone	6	L	1	1	1	1	1	1	1
Ethyl acrylate	4	L	0	1	1	1	1	1	1
Methyl methacrylate	4	H	1	1	1	0	2	1	1
n-Heptane	1	L	1	0	0	0	0	3	0
n-Propyl acetate	4	L	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	L	0	0	0	0	0	1	0
Piperidine	8	H	0	0	0	0	0	0	0
Pyridine	8	L	1	0	0	0	0	1	0
Toluene	9	L	1	1	1	1	1	1	1
2-Methylthiophene	13	H	1	1-	1	1	1	1	1
n-Butyl acetate	4	H	1	1	1	1	1	1	1
n-Octane	1	L	1	1	0	0	0	5	3
Tetrachloroethylene	10	L	1	1	1	1	1	1	1
Di-n-butyl ether	5	L	0	0	1	0	1	0	1
n-Butyl acrylate	4	L	1	1	1	1	1	1	0
Styrene	9	H	1	1	1	1	1	1	1
n-Heptaldehyde	3	L	0	0	1	0	0	0	2
o-Xylene	9	L	1	1-	1-	0	2-	1	3-
1,1,2,2-Tetrachloroethane	10	L	1	1	1	1	1	1	1

(continued)

Table A17 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
n-Ethyltoluene	9	H	1	1	2-	2	0	1	0
Benzonitrile	7	L	1	0	2	0	1	1	2
p-Ethyltoluene	9	L	1	3-	0	0	0	0	0
1,3,5-Trimethylbenzene	9	H	0	1-	1-	1	1-	1	1-
Butyl methacrylate	4	L	1	1	2	0	0	1	1
Phenol	15	L	1	1	1	1	1	1	0
p-Dichlorobenzene	11	H	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1	1	0	0	1	1
p-Cresol	15	L	1	1	1-	1-	1-	1-	1-
m-Cresol	15	L	0	1	0	0	0	0	0
Nitrobenzene	8	L	0	0	0	0	0	1	0
p-Tolualdehyde	12	H	1	1	1	1	1	1	1
2-Methylbenzofuran	5	H	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	1	0	0	1	1
Naphthalene	9	H	1	2	2	1	1	1	1
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	H	1	1	1	0	0	1	1
2-Benzothiazole	13	L	0	0	0	0	0	0	0
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	0	1
o-Chloronitrobenzene	11	H	1	1-	1-	1-	1-	1	1
Quinoline	8	L	0	0	0	0	0	1	0

Footnotes - Table A17

[a]Interpretation by an experienced person.

[b]RTI Mass Spectral Search System.

[c]Fouirer Transformed Mass Spectral Search.

[d]Mass spectral search software on Incos Data System (Finnigan Corp.).

[e]No Reindfleisch deconvolution pretreatment.

[f]Reindfleisch deconvolution pretreatment of data prior to search.

[g]M = medium, L = low, H = high.

Table A18. CHEMICALS IDENTIFIED IN MIXTURE NO. 18

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Acrolein	3	L[g]	0	0	0	0	0	0	0
Acetonitrile	7	H	0	0	0	5	0	0	0
Propionaldehyde	3	L	1	0	0	0	0	0	0
Acetone	6	L	0	0	2	0	1	0	1
Diethyl ether	5	L	0	0	0	0	0	1	1
Ethanol	2	L	0	0	0	0	0	0	0
Acrylonitrile	7	L	0	0	0	0	0	0	0
Vinylidene chloride	10	H	1	1	1	1-	1-	1	1
Methylene chloride	10	L	1	1	1	1	1	1	1
t-Butanol	2	L	1	0	1	1	0	1	1
2-Methylfuran	5	L	1	1-	1-	1	1-	1	1
Perfluorobenzene	11	L	0	0	0	0	0	0	0
n-Hexane	1	H	1	1	1	1	1	1	1
Ethyl acetate	4	L	1	1	1	1	1	1	0
Chloroform	10	L	1	2	2	1	2	1	1
Perfluorotoluene	11	L	1	1	1	0	0	1	1
1,2-Dichloroethane	10	L	1	1	2	1	1	1	1
1,1,1-Trichloroethane	10	H	1	1	1	1	1	1	1
Benzene	9	L	1	1	1	1	1	1	1
Thiophene	13	L	1	1	1	1	5	1	1
Pyrrolidine	8	L	0	0	0	0	0	0	0

(continued)

Table A18 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
2-Pentanone	6	L	1	4	3	0	3	1	1
Acetic acid	14	L	1	1	1	1	1	1	1
1,2-Dichloropropane	10	H	1	1	1-	1	1	1	1
3-Pentanone	6	L	1	1	1	1	1	1	1
Ethyl acrylate	4	L	0	3	1	2	1	1	1
Methyl methacrylate	4	L	1	1	0	0	0	0	1
n-Heptane	1	L	1	1	0	4	0	1	1
n-Propyl acetate	4	H	1	1	1	1	1	1	1
α-Methylbutyronitrile	7	L	0	0	1-	3	1-	1	3
Piperidine	8	L	0	0	0	0	0	0	0
Pyridine	8	L	1	1	4	1	0	1	1
Toluene	9	L	1	1	1	1	1	1	1
2-Methylthiophene	13	L	1	1	1-	1	1	1-	1-
n-Butyl acetate	4	L	1	0	1	0	1	1	1
n-Octane	1	L	0	0	0	0	0	4	0
Tetrachloroethylene	10	H	1	1	1	1	1	1	1
Di-n-butyl ether	5	L	0	1	1	1-	2	1	3
n-Butyl acrylate	4	L	0	0	0	0	0	1	0
Styrene	9	L	1	1	1	1	1	1	1
n-Heptaldehyde	3	L	0	0	0	0	0	0	1
o-Xylene	9	H	1	1-	1-	1-	1-	1-	1-
1,1,2,2-Tetrachloroethane	10	L	1	1	1	1	1	1	1

(continued)

Table A18 (cont'd.)

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
m-Ethyltoluene	9	L	1	1-	3	1	2	1-	0
Benzonitrile	7	L	0	0	0	0	0	0	0
p-Ethyltoluene	9	H	1	1-	1-	1	0	1-	1-
1,3,5-Trimethylbenzene	9	L	0	1-	1-	1-	1-	1	1-
Butyl methacrylate	4	L	1	2	2	0	0	1	1
Phenol	15	H	1	1	4	1	1	1	1
p-Dichlorobenzene	11	L	1	1-	1-	1-	1-	1	1
n-Decane	1	L	1	1	2	0	0	1	1
p-Cresol	15	L	1	0	0	1	1	1	0
m-Cresol	15	H	1	1	1	1-	0	1	1
Nitrobenzene	8	L	1	1	0	1	5	0	0
p-Tolualdehyde	12	L	1	2-	1-	2-	4-	1	1
2-Methylbenzofuran	5	L	1	1	1	1	1	1	1
n-Undecane	1	L	1	1	1	0	0	0	1
Naphthalene	9	L	1	1	2	1	2	1	1
1-Benzothiophene	13	L	1	1	1	1	1	1	1
n-Dodecane	1	L	1	1	1	0	0	1	1
2-Benzothiazole	13	L	1	2	2	1	0	1	1
Hexachloro-1,3-butadiene	10	L	1	1	1	1	1	1	1
o-Chloronitrobenzene	11	L	1	0	1-	0	1-	0	0
Quinoline	8	H	1	2	2	3	3	2	0

Footnotes - Table A18 (cont'd.)

[a]Interpretation by an experienced person.

[b]RTI Mass Spectral Search System.

[c]Fouirer Transformed Mass Spectral Search.

[d]Mass spectral search software on Incos Data System (Finnigan Corp.).

[e]No Reindfleisch deconvolution pretreatment.

[f]Reindfleisch deconvolution pretreatment of data prior to search.

[g]M = medium, L = low, H = high.

Table A19. CHEMICALS IDENTIFIED IN MIXTURE NO. 19

Chemical	Group	Level	Manual[a]	MSSS[b]		MSFS[c]		Incos[d]	
				ND[e]	D[f]	ND	D	ND	D
Methanol	2	M[g]	0	0	0	0	0	0	0
Methyl bromide	10	H	1	1	1	1	1	1	1
Vinyl bromide	10	H	1	1	1	1	1	1	1

[a] Interpretation by an experienced person.

[b] RTI Mass Spectral Search System.

[c] Fourier Transformed Mass Spectral Search.

[d] Mass spectral search software on Incos Data System (Finnigan Corp.).

[e] No Reindfleisch deconvolution pretreatment.

[f] Reindfleisch deconvolution pretreatment of data prior to search.

[g] M = medium, L = low, H = high.

APPENDIX B

SUMMARY OF RESULTS FOR EACH ENVIRONMENTAL SAMPLE SUBJECTED TO MANUAL AND AUTOMATED ALGORITHM IDENTIFICATION

Table B1. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 1 (LOCATION-1, VOL-L)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
52	ethyl chloride	10	1	1	0	1
63	trichlorofluoromethane	10	0	0	1	1
74	acetone	6	1	0	1	1
83	1,1,2-trichloro-1,2,2-trifluoroethane	10	1	1	1	1
109	saturated hydrocarbon	1	1	0	1	1
139	hexafluorobenzene	11	1	1	1	1
168	methylcyclopentane	1	1	0	0	0
178	perfluorotoluene	11	1	1	1	1
181	1,1,1-trichloroethane	10	1	0	1	1
201	benzene	9	1	1	1	1
206	carbon tetrachloride & saturated hydrocarbon	10	1	0	0	1
210	cyclohexane	1	1	0	0	1
226	C_7H_{16} isomer	1	0	0	0	1
238	C_7H_{16} isomer	1	1	1	0	1
277	n-heptane	9	1	1	1	1
307	methylcyclohexane	1	0	1	0	1
337	saturated hydrocarbon	1	1	0	0	1
359	unsaturated hydrocarbon	1	0	0	0	0
374	toluene	9	1	1	1	0
387	unsaturated hydrocarbon	1	0	0	0	0
400	acetic acid	14	1	1	1	1
417	saturated hydrocarbon and unsaturated hydrocarbon	1	1	0	0	1
447	C_8H_{16} isomer	1	0	1	0	1
470	tetrachloroethylene and C_8H_{16} isomer	10	1	1	1	0
477	n-octane	1	1	0	1	1
531	C_9H_{20} isomer	1	0	0	0	0
539	chlorobenzene	11	1	1	1	1
581	pentanoic acid	14	0	0	0	0
585	xylene isomer	9	0	1	1	1
606	xylene isomer	9	1	1	1	1
637	saturated & unsaturated hydrocarbons	1	0	0	0	0
643	styrene	9	1	0	1	1
652	xylene isomer	9	1	1	1	1
658	saturated hydrocarbon	1	0	0	0	0
672	saturated hydrocarbon	1	1	1	0	1
698	saturated hydrocarbon	1	0	1	0	0
702	saturated hydrocarbon	1	1	1	0	1
741	saturated hydrocarbon	1	1	1	0	1
763	saturated hydrocarbon	1	0	0	0	0
771	benzaldehyde	12	0	0	1	1
811	C_3H_7-benzene isomer	9	1	1	1	1
813	benzonitrile	7	0	0	1	0
829	C_3H_7-benzene isomer	9	1	0	1	0
847	saturated hydrocarbon	1	0	1	0	1

(continued)

Table B1 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
858	unsaturated hydrocarbon	1	0	0	0	0
877	saturated hydrocarbon	1	1	1	0	1
887	C_3H_7-benzene isomer	9	1	1	1	1
890	phenol	15	0	0	1	0
897	saturated hydrocarbon	1	1	0	0	0
917	saturated hydrocarbon	1	1	1	0	0
927	saturated hydrocarbon	1	1	1	0	1
937	saturated hydrocarbon	1	1	1	0	1
949	C_3H_7-benzene isomer	9	0	0	0	0
956	octamethyl cyclotetrasiloxane	1	0	0	0	0
959	dichlorobenzene isomer	11	1	1	1	1
1016	acetophenone	6	1	1	1	1
1036	C_4H_9-benzene isomer	9	0	0	0	0
1086	o-cresol	15	1	1	1	1
1091	C_4H_9-benzene isomer	9	0	0	0	0
1155	saturated hydrocarbon	1	1	1	1	1
1165	C_4H_9-benzene isomer	9	0	0	0	0
1207	ethylphenol isomer	15	0	0	1	0
1228	dimethylphenol isomer	15	0	1	0	1
1269	ethylphenol isomer	15	1	1	0	1
1274	naphthalene	9	0	0	0	1
1294	decamethylcyclopentasiloxane	1	0	0	0	0
1330	n-decanal	3	1	1	0	0
1341	benzothiazole	13	0	0	1	0
1492	methylnaphthalene isomer	9	0	0	0	0
1638	biphenyl	9	0	0	0	0

Table B2. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 1 (LOCATION-2, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
39	chloromethane	10	1	1	0	1
52	ethylchloride	10	1	1	0	1
63	trichlorofluoromethane	10	0	0	1	1
71	acetone	6	0	0	1	0
81	dichloromethane	10	1	1	0	1
84	1,1,2-trichloro-1,2,2-trifluoromethane	10	1	1	0	1
110	2-methylpentane	1	1	1	0	1
122	3-methylpentane	1	1	1	0	1
138	hexafluorobenzene	11	1	1	1	0
140	n-hexane	1	1	1	1	1
148	chloroform	10	0	0	0	0
169	methylcyclopentane	1	0	0	0	1
173	1,2-dichloroethane	10	1	1	1	1
179	perfluorotoluene	11	1	1	1	1
182	1,1,1-trichloroethane	10	0	0	1	0
201	benzene	9	0	0	1	1
207	carbon tetrachloride and saturated hydrocarbon	10	1	1	0	1
211	cyclohexane	1	1	1	0	0
228	C_7H_{16} isomer	1	1	1	0	1
230	C_7H_{14} isomer	1	1	0	0	0
241	3-methylhexane	1	1	1	0	0
249	C_7H_{14} isomer	1	0	0	0	0
258	trichloroethylene	10	0	0	0	0
261	saturated hydrocarbon	1	1	1	0	0
281	n-heptane	1	0	0	1	1
285	methyl methacrylate or $C_5H_8O_2$ isomer	4	1	1	1	1
313	methylcyclohexane	1	1	1	0	1
319	saturated hydrocarbon	1	1	1	0	1
337	C_7H_{14} isomer	1	0	0	0	0
344	C_8H_{18} isomer	1	1	1	0	1
354	C_8H_{16} isomer	1	0	0	0	0
357	C_8H_{18} isomer	1	1	1	0	1
363	C_8H_{16} isomer	1	0	0	0	0
379	tetramethyllead	1	1	1	0	1
384	toluene	9	1	1	1	0
389	acetic acid	14	0	0	0	0
399	unsaturated hydrocarbon	1	1	0	0	1
412	C_8H_{18} isomer	1	1	1	0	1
426	C_8H_{16} isomer	1	1	1	0	0
428	C_8H_{18} isomer	1	1	1	0	1
428	C_8H_{18} isomer	1	1	1	0	1
437	dibromoethane isomer	10	1	1	0	1
450	saturated hydrocarbon	1	1	1	0	1
456	C_8H_{16} isomer	1	0	0	0	0

(continued)

Table B2 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			MD	D	MD	D
468	C_8H_{16} isomer	1	0	0	0	0
479	tetrachloroethylene	10	1	1	1	1
486	n-octane	1	1	1	1	1
516	isopropyl crotonate or $C_7H_{12}O_2$ isomer	4	0	0	0	1
539	C_9H_{20} isomer	1	0	0	0	1
548	chlorobenzene	11	1	1	1	1
560	C_9H_{18} isomer	1	0	0	0	0
569	saturated hydrocarbon	1	1	1	0	1
592	ethylbenzene	9	0	1	1	1
612	xylene isomer	9	1	1	1	1
635	C_9H_{20} isomer	1	1	1	0	1
650	C_9H_{20} isomer	1	0	0	0	0
652	styrene	9	1	1	1	1
658	xylene isomer	9	1	1	1	1
663	saturated hydrocarbon	1	1	1	0	1
670	C_3H_7-cyclohexane isomer	1	0	0	0	0
676	saturated hydrocarbon	1	1	1	0	1
702	C_9H_{20} isomer	1	0	0	0	0
706	n-nonane	1	1	1	0	1
729	isopropylbenzene	9	0	1	0	1
764	C_9H_{18} isomer	1	1	1	0	1
775	benzaldehyde	3	0	0	1	1
787	saturated hydrocarbon	1	1	0	0	1
797	n-propylbenzene	9	1	1	0	1
815	C_3H_7-benzene isomer	9	1	1	1	1
833	C_3H_7-benzene isomer	9	1	1	1	1
851	saturated hydrocarbon	1	1	1	0	1
855	C_3H_7-benzene isomer	9	1	1	1	1
871	saturated hydrocarbon	1	1	1	0	1
879	saturated hydrocarbon	1	1	1	0	1
884	methylstyrene isomer or C_9H_{10} isomer	9	0	0	0	0
888	C_3H_7-benzene isomer	9	1	1	1	1
893	phenol	15	0	0	1	0
898	$C_{11}H_{24}$ isomer	1	1	1	0	1
910	dichlorobenzene isomer	11	0	0	1	0
918	saturated hydrocarbon	1	0	1	0	1
928	saturated hydrocarbon	1	1	1	0	0
937	n-decane	1	1	1	1	1
948	C_3H_7-benzene isomer	9	1	1	1	1
954	C_4H_9-benzene isomer and octamethylcyclotetrasiloxane	9	1	0	0	0
958	dichlorobenzene isomer	11	1	1	1	1
960	C_4H_9-benzene isomer	9	1	1	0	0
971	methylstyrene isomer or C_9H_{10} isomer	9	0	0	0	1
989	saturated hydrocarbon	1	1	1	0	1

Table B2 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
996	saturated hydrocarbon	1	1	1	0	1
1013	acetophenone	6	1	1	1	1
1026	C_4H_9-benzene isomer	9	1	1	0	0
1032	C_4H_9-benzene isomer	9	1	1	0	1
1044	nitrobenzene	8	1	1	1	1
1048	C_4H_9-benzene isomer	9	1	1	0	0
1057	saturated hydrocarbon	1	0	1	0	1
1071	C_4H_9-benzene isomer	9	0	1	0	1
1082	cresol isomer	15	1	1	1	1
1083	ethylstyrene isomer or $C_{10}H_{12}$ isomer	9	0	0	0	0
1087	C_4H_9-benzene isomer	9	1	1	0	1
1150	u-undecane	1	1	1	1	1
1154	C_4H_9-benzene isomer	9	0	0	0	0
1161	C_4H_9-benzene isomer	9	1	1	0	1
1206	o-nitrotoluene	8	1	1	0	0
1224	dimethylphenol isomer	15	1	1	0	1
1260	trichlorobenzene isomer	11	0	0	1	0
1267	ethyl phenol isomer	15	0	1	0	0
1271	naphthalene	9	0	0	1	1
1278	C_2H_5-phenol isomer	15	1	1	0	1
1313	p-nitrotoluene	8	1	1	0	1
1332	1-chloro-3-nitrobenzene	8	1	1	0	1
1348	p-chloronitrobenzene	8	1	1	1	1
1353	n-dodecane	1	0	0	1	0
1487	methylnaphthalene isomer	9	1	1	0	1
1541	saturated hydrocarbon	1	1	1	0	0
1635	biphenyl	9	0	0	0	0

Table B3. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLES FROM SITE NO. 1 (LOCATION-1, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
52	ethyl chloride	10	1	1	0	1
63	trichlorofluoromethane	10	0	0	0	1
69	acetone	6	0	0	0	0
83	1,1,2-trichloro-1,2,2-trifluoromethane	10	1	1	0	0
108	2-methylpentane or C_6H_{14} isomer	1	1	1	0	1
120	3-methylpentane or C_6H_{14} isomer	1	1	1	0	1
135	hexafluorobenzene	11	1	1	1	0
138	n-hexane	1	1	0	1	1
146	chloroform	10	0	0	1	0
167	methylcyclopentane	1	1	1	0	1
171	1,2-dichloroethane	10	0	0	1	0
176	perfluorotoluene	11	1	1	1	1
178	1,1,1-trichloroethane	10	1	1	1	1
198	benzene	9	1	1	1	1
203	saturated hydrocarbon	1	1	1	0	1
204	carbon tetrachloride	10	0	0	0	0
207	cyclohexane	1	1	1	0	0
221	C_7H_{16} isomer	1	1	0	0	1
227	C_7H_{14} isomer	1	1	0	0	0
235	3-methylhexane	1	1	1	0	0
243	C_7H_{14} isomer	1	0	0	0	0
253	trichloroethylene	10	0	0	1	0
254	saturated hydrocarbon	1	1	0	0	1
274	n-heptane	1	1	1	1	1
276	methyl methacrylate or $C_5H_8O_2$ isomer	4	0	0	1	0
304	methylcyclohexane	1	1	1	0	1
330	C_8H_{18} isomer	1	1	1	0	1
334	C_8H_{18} isomer	1	1	1	0	1
367	acetic acid	14	0	0	1	0
372	toluene	9	1	1	1	1
398	C_8H_{18} isomer	1	1	0	0	0
423	dibromoethane isomer	10	0	0	0	0
437	saturated hydrocarbon	1	0	0	0	0
456	C_8H_{16} isomer	1	0	0	0	0
466	tetrachloroethylene	10	1	0	1	1
474	n-octane	1	1	1	1	1
536	chlorobenzene	11	1	1	1	1
558	saturated hydrocarbon	1	1	0	0	1
583	C_2H_5-benzene isomer	9	1	1	1	1
604	C_2H_5-benzene isomer	9	1	1	1	1
610	phenylacetylene	9	0	0	0	0
622	cyclohexanone	6	0	0	1	1
626	C_9H_{20} isomer	1	1	0	0	1

(continued)

Table B3 (cont'd.)

Scan No.	Chemical	Class No.	MSSS ND	MSSS D	Incos ND	Incos D
644	styrene	9	1	1	1	1
653	C_2H_5-benzene isomer	9	1	1	1	1
667	1-methyl-4-ethylcyclohexane isomer	1	0	0	0	0
674	$C_{10}H_{22}$ isomer	1	0	1	0	0
701	saturated hydrocarbon	1	1	1	0	0
706	C_9H_{20} isomer	1	1	0	0	1
729	isopropylbenzene	9	1	0	0	0
745	saturated hydrocarbon	1	1	1	0	1
746	propylcyclohexane isomer	1	1	0	0	0
767	saturated hydrocarbon	1	1	0	0	1
775	benzaldehyde	12	0	0	1	1
787	saturated hydrocarbon	1	1	0	0	1
797	n-propylbenzene	9	0	0	0	1
816	C_3H_7-benzene isomer	9	1	0	1	1
834	C_3H_7-benzene isomer	9	1	0	1	1
852	saturated hydrocarbon	1	1	0	0	1
881	saturated hydrocarbon	1	1	0	0	1
886	methyl styrene isomer or C_9H_{10} isomer	9	0	1	0	0
891	C_3H_7-benzene isomer	9	1	0	1	1
896	phenol	15	0	0	1	0
901	saturated hydrocarbon	1	0	0	1	0
913	dichlorobenzene isomer	11	0	0	1	0
920	saturated hydrocarbon	1	0	1	0	0
930	$C_{10}H_{22}$ isomer	1	0	0	0	0
940	n-decane	1	1	0	0	1
951	C_3H_7-benzene isomer	9	1	0	1	1
957	C_4H_9-benzene isomer	9	0	0	0	0
961	dichlorobenzene isomer	11	1	1	1	1
974	methyl styrene isomer or C_9H_{10} isomer	9	1	0	0	0
984	limonene or $C_{10}H_{16}$ isomer	1	1	0	0	0
992	saturated hydrocarbon	1	1	1	0	1
1016	acetophenone	6	1	1	1	1
1028	C_4H_9-benzene isomer	9	1	0	0	1
1035	C_4H_9-benzene isomer	9	1	0	0	1
1052	C_4H_9-benzene isomer	9	1	0	0	0
1075	C_4H_9-benzene isomer	9	0	0	0	0
1085	cresol isomer	15	1	1	1	1
1086	ethylstyrene isomer	9	0	0	0	1
1091	C_4H_9-benzene isomer	9	1	0	0	0
1155	n-undecane	1	1	0	1	1
1165	C_4H_9-benzene isomer	9	1	0	0	1
1210	o-nitrotoluene	8	1	0	0	0
1218	ethylstyrene isomer	9	1	0	0	1
1229	dimethylphenol isomer	15	1	1	0	1

(continued)

Table B3 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
1252	C_5H_{11}-benzene isomer	9	0	0	0	0
1274	naphthalene	9	0	0	1	1
1281	ethyl phenol isomer	15	0	1	0	0
1358	saturated hydrocarbon	1	1	0	0	1
1483	methyl naphthalene isomer	9	1	0	0	1
1511	methyl naphthalene isomer	9	1	0	0	1
1537	saturated hydrocarbon	1	1	1	0	1
1626	biphenyl	9	1	0	0	0

Table B4. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 2 (LOCATION-1, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
66	trichlorofluoromethane	10	0	0	1	1
74	acetone	6	0	0	1	0
139	n-hexane	1	0	0	0	0
141	hexafluorobenzene	11	1	1	1	1
152	ethyl acetate	4	2	1	1	1
179	perfluorotoluene	11	1	0	1	1
182	1,1,1-trichloroethane	10	1	0	0	1
202	benzene	9	1	1	1	1
227	1-butanol	2	0	0	1	0
258	trichloroethylene	10	1	0	0	1
278	n-heptane	1	1	1	1	1
282	methyl methacrylate	4	1	0	0	1
311	methylcyclohexane	1	1	1	1	1
340	saturated hydrocarbon	1	1	0	0	0
352	saturated hydrocarbon	1	1	1	0	1
380	toluene	9	1	1	1	1
392	unsaturated hydrocarbon	1	0	0	0	0
409	acetic acid	14	1	1	1	1
422	C_8H_{18} isomer	1	0	0	1	1
438	unsaturated hydrocarbon	1	0	0	0	0
455	C_8H_{16} isomer	1	1	0	0	1
476	tetrachloroethylene	10	1	1	0	1
481	n-octane	1	1	1	1	1
543	chlorobenzene	11	1	1	0	1
547	hexamethylcyclotrisiloxane	1	0	0	1	1
565	saturated hydrocarbon	1	1	0	1	1
590	ethylbenzene	9	1	0	1	1
610	xylene isomer	9	1	1	1	1
617	phenylacetylene	9	1	1	0	0
634	C_9H_{20}isomer	1	1	0	1	1
645	C_9H_{20}isomer	1	1	0	0	0
653	styrene	9	0	1	0	0
663	xylene isomer	9	1	1	1	1
684	saturated hydrocarbon	1	1	0	1	1
715	n-nonane	1	1	1	1	1
740	C_3H_7-benzene isomer	9	1	0	0	1
757	saturated hydrocarbon	1	1	0	1	1
791	benzaldehyde	12	1	0	1	1
814	C_3H_7-benzene isomer	9	1	0	0	1
833	C_3H_7-benzene isomer	9	1	0	1	1
835	benzonitrile	7	1	0	0	0
852	C_3H_7-benzene isomer	9	1	0	0	1
855	saturated hydrocarbon	1	0	0	0	0

(continued)

Table B4 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
870	saturated hydrocarbon	1	1	1	1	1
878	n-butyl methacrylate	4	1	1	1	1
891	saturated hydrocarbon	1	1	1	1	1
893	phenol	15	0	0	0	0
900	saturated hydrocarbon	1	1	0	0	0
909	C_3H_7-benzene isomer	9	1	0	0	1
919	n-octanal	3	1	1	0	1
939	saturated hydrocarbon	1	1	0	0	1
959	saturated hydrocarbon	1	1	1	0	1
971	C_3H_7-benzene isomer	9	1	0	0	0
993	octamethylcyclotetrasiloxane	1	0	0	1	0
1039	acetophenone	6	0	1	1	1
1058	C_4H_9-benzene isomer	9	1	1	0	1
1083	saturated hydrocarbon	1	1	1	0	1
1103	saturated hydrocarbon	1	1	1	0	1
1112	C_4H_9-benzene isomer	9	1	0	0	1
1127	saturated hydrocarbon	1	1	1	0	1
1143	n-nonanal	3	1	1	1	1
1174	saturated hydrocarbon	1	1	1	1	1
1187	C_4H_9-benzene isomer	9	1	0	0	1
1296	naphthalene	9	0	0	0	0
1315	decamethylcyclopentasiloxane	1	0	0	0	0
1352	n-decanal	3	1	1	1	1
1378	n-dodecane	1	0	1	0	0
1512	methylnaphthalene isomer	1	1	1	0	1
1566	n-tridecane	1	0	0	0	0
1636	alkyl butyrate	4	1	0	0	0
1643	silane compound	1	0	1	0	1
1667	isobutyrate compound	4	0	0	1	1
1739	saturated hydrocarbon	1	1	1	0	1
1887	saturated hydrocarbon	1	1	1	0	1
1976	diethyl phthalate	4	1	0	1	1
2026	2,2,4-trimethylpenta-1,3-diol di-isobutyrate	4	0	0	0	0

Table B5. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 2 (LOCATION-1, VOL-L)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
66	trichlorofluoromethane	10	0	0	0	0
74	acetone	6	1	0	0	0
120	n-hexane	1	0	0	0	0
136	methylfuran isomer	5	0	0	1	1
140	hexafluorobenzene	11	1	1	1	1
150	ethyl acetate	4	1	1	1	0
178	perfluorotoluene	11	1	1	1	1
180	1,1,1-trichloroethane	10	0	1	0	1
200	benzene	9	1	0	1	1
225	1-butanol	2	1	1	1	1
233	2-pentanone	6	0	0	1	1
248	3-pentanone	6	1	1	1	1
272	p-diozane	5	0	0	0	0
276	n-heptane	1	0	0	0	1
287	n-propyl acetate	4	1	0	0	0
309	methylcyclohexane	1	1	1	0	1
352	C_8H_{18} isomer	1	0	1	0	1
380	toluene	9	1	1	0	0
393	unsaturated hydrocarbon	1	0	1	0	0
406	C_8H_{18} isomer	1	0	1	0	0
422	C_8H_{18} isomer	1	0	0	0	1
437	unsaturated hydrocarbon	1	0	0	0	1
454	C_8H_{16} isomer	1	1	1	1	1
479	n-octane	1	1	1	1	1
488	C_8H_{16} isomer	1	1	1	0	1
508	acetic acid	14	1	1	1	1
545	hexamethylcyclotrisiloxane	1	0	0	0	1
562	saturated hydrocarbon	1	0	0	0	0
588	ethylbenzene	9	0	0	1	1
613	xylene isomer	9	1	0	1	1
643	saturated hydrocarbon	1	0	0	0	1
651	styrene	9	1	1	0	0
660	xylene isomer	9	1	1	0	1
671	butyl acrylate	4	1	1	1	1
682	saturated hydrocarbon	1	0	1	0	1
716	n-nonane	1	1	1	1	1
759	saturated hydrocarbon	1	0	1	1	1
793	benzaldehyde	12	1	0	1	1
840	C_3H_7-benzene isomer	9	1	0	1	0
843	C_3H_7-benzene isomer	9	1	0	0	0
873	saturated hydrocarbon	1	1	1	1	1
877	C_3H_7-benzene isomer	9	1	1	0	1
903	saturated hydrocarbon	1	0	1	0	1
908	methylstyrene isomer	9	0	0	0	0

(continued)

Table B5 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
912	C_3H_7-benzene isomer	9	0	0	0	0
916	phenol	15	0	0	0	0
943	2-octanol	2	1	1	1	1
963	saturated hydrocarbon	1	1	1	0	1
975	C_3H_7-benzene isomer	9	0	0	0	0
984	octamethylcyclotetrasiloxane	1	0	0	0	0
1010	2-ethyl-1-hexanol	2	0	0	1	1
1025	saturated hydrocarbon	1	1	1	0	1
1045	acetophenone	6	1	1	1	1
1051	tolualdehyde isomer	12	0	0	0	0
1078	tolualdehyde isomer	12	1	1	0	1
1114	cresol isomer	15	1	1	1	0
1152	n-nonanal	3	1	1	0	1
1183	saturated hydrocarbon	1	1	1	0	1
1252	dimethyl phenol isomer	15	1	1	1	0
1256	dimethyl phenol isomer	15	1	1	1	1
1275	C_4H_9-benzene isomer	9	0	0	0	0
1297	ethyl phenol isomer	15	1	1	0	1
1300	C_4H_9-benzene isomer	9	0	0	0	0
1305	naphthalene	9	0	0	0	1
1311	C_2H_5-phenol isomer	15	1	1	0	1
1361	n-decanal	3	0	1	1	1
1522	methylnaphthalene isomer	9	0	1	0	1
1575	n-tridecane	1	0	0	0	0
1676	isobutyrate compound	4	1	1	1	1
1747	saturated hydrocarbon	1	1	1	0	1

Table B6. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 2 (LOCATION-2, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
73	trichlorofluoromethane	10	0	0	0	1
76	acetone	6	0	0	0	0
143	hexafluorobenzene	11	1	1	1	1
170	methylcyclopentane	1	0	0	0	0
180	perfluorotoluene	11	1	1	1	1
183	1,1,1-trichloroethane	10	0	0	1	1
202	benzene	0	1	1	1	1
238	saturated hydrocarbon	1	1	1	0	1
244	1,2-dichloropropane	10	0	0	1	1
258	trichloroethylene	10	1	0	0	1
278	n-heptane	1	1	1	1	1
310	methylcyclohexane	1	1	1	1	1
326	4-methyl-2-pentanone	6	0	0	0	1
379	toluene	9	1	1	0	0
405	saturated hydrocarbon	1	1	0	1	0
421	saturated hydrocarbon	1	1	0	1	1
438	saturated hydrocarbon	1	0	0	0	0
459	acetic acid	14	1	0	1	1
474	tetrachloroethylene	10	1	1	1	1
480	n-octane	1	1	1	1	1
545	hexamethylcyclotrisiloxane	1	0	0	0	1
563	saturated hydrocarbon	1	1	0	1	1
574	2-hexanone	6	0	0	1	0
588	ethylbenzene	9	0	0	1	1
609	xylene isomer	9	1	1	1	1
615	phenylacetylene	9	1	0	0	0
632	saturated hydrocarbon	1	1	0	1	1
643	saturated hydrocarbon	1	0	0	0	1
651	styrene	9	1	1	1	0
662	xylene isomer	9	1	1	1	1
668	saturated hydrocarbon	1	1	1	1	1
683	saturated hydrocarbon	1	1	1	0	1
712	n-nonane	1	0	1	0	0
735	C_3H_7-benzene isomer	9	1	1	1	1
751	saturated hydrocarbon	1	1	1	1	1
783	benzaldehyde	12	0	0	1	1
804	n-propylbenzene	9	0	1	1	1
823	C_3H_7-benzene isomer	9	1	1	1	1
841	C_3H_7-benzene isomer	9	1	1	1	1
860	saturated hydrocarbon	1	1	1	1	1
866	methylstyrene isomer	9	1	0	0	0
868	phenol	15	0	0	0	0
890	saturated hydrocarbon	1	1	1	1	1
900	C_3H_7-benzene isomer	9	1	1	1	1
910	saturated hydrocarbon	1	1	1	1	1

(continued)

Table B6 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			MD	D	MD	D
929	C_8H_{14} isomer	1	1	0	0	0
931	saturated hydrocarbon	1	1	1	0	0
940	saturated hydrocarbon	1	0	1	0	0
946	octamethylcyclotetrasiloxane	1	0	0	0	0
950	n-decane	1	0	0	0	0
963	C_3H_7-benzene isomer	9	1	1	0	1
970	octamethylcyclotetrasiloxane	1	0	0	0	1
983	saturated hydrocarbon	1	1	0	0	1
987	methylstyrene isomer	9	0	1	0	0
1013	saturated hydrocarbon	1	1	1	1	1
1032	acetophenone	6	1	1	1	1
1053	C_4H_9-benzene isomer	9	1	1	0	1
1078	saturated hydrocarbon	1	1	1	1	1
1093	C_4H_9-benzene isomer	9	0	1	0	1
1100	saturated hydrocarbon	1	1	1	1	0
1110	C_4H_9-benzene isomer	9	1	1	1	1
1141	n-nonanal	3	0	0	0	0
1174	saturated hydrocarbon	1	1	1	0	1
1178	C_4H_9-benzene isomer	9	1	1	0	1
1186	C_4H_9-benzene isomer	9	1	1	0	1
1248	benzoic acid	14	0	0	0	0
1286	C_2H_5-phenol isomer	15	0	0	0	0
1296	naphthalene	9	0	0	0	1
1315	decamethylcyclopentasiloxane	1	0	0	0	1
1353	n-decanal	3	1	1	0	1
1379	n-dodecane	1	1	1	0	0
1441	saturated hydrocarbon	1	0	0	0	0
1516	methylnaphthalene isomer	9	1	1	0	1
1544	methylnaphthalene isomer	9	1	0	0	0
1569	n-tridecane	1	0	0	0	0
1639	alkyl butyrate	4	1	1	0	0
1646	silane compound	1	1	0	0	1
1671	isobutyrate compound	4	0	0	1	1
1744	saturated hydrocarbon	1	1	1	1	0
1841	saturated hydrocarbon	1	0	0	1	1
1905	saturated hydrocarbon	1	1	1	1	1
1997	phthalate	4	1	0	1	1

Table B7. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 4 (LOCATION-1, VOL-H)

Scan No.	Chemical	Class No.	MSSS ND	MSSS D	Incos ND	Incos D
70	acetone	5	0	0	0	0
76	trichlorofluoromethane	10	0	0	1	1
92	carbon disulfide	13	0	0	0	0
116	2-methylpentane	1	0	1	1	1
128	3-methylpentane and methyl ethyl ketone	1	0	1	1	1
144	n-hexane	1	0	1	0	0
146	hexafluorobenzene	11	1	1	1	1
157	ethyl acetate	4	1	1	1	1
172	$C_6H_{14}O$ isomer	4	0	0	0	0
182	perfluorotoluene	11	1	1	1	1
185	1,1,1-trichloroethane	10	1	0	1	1
204	benzene	9	1	1	1	1
234	n-butyl alcohol	2	0	0	1	0
259	trichloroethylene	10	0	0	0	1
279	n-heptane	1	1	1	1	1
296	saturated hydrocarbon	1	0	0	0	0
310	methylcyclohexane	1	1	1	1	1
338	saturated hydrocarbon	1	0	0	1	0
377	toluene	9	1	1	1	1
403	C_8H_{18} isomer	1	0	0	1	1
417	C_8H_{16} isomer and saturated hydrocarbon	1	0	1	1	0
432	C_8H_{18} isomer	1	0	0	0	0
436	unsaturated hydrocarbon	1	0	0	0	0
449	unsaturated hydrocarbon	1	0	0	0	0
470	acetic acid	14	1	0	1	0
474	n-octane	1	1	0	1	0
480	n-butyl acetate	4	0	0	1	0
536	hexamethylcyclotrisiloxane	1	0	0	1	0
578	ethylbenzene	9	1	1	1	1
599	xylene isomer	9	1	1	1	0
605	phenylacetylene	9	0	0	0	0
622	saturated hydrocarbon	1	0	0	1	0
632	saturated hydrocarbon	1	0	0	0	0
651	xylene isomer	9	1	0	0	0
657	saturated hydrocarbon	1	0	0	1	0
672	saturated hydrocarbon	1	0	0	1	0
699	saturated hydrocarbon	1	0	0	0	0
703	n-nonane	1	1	0	0	0
739	saturated hydrocarbon	1	1	1	1	1
770	benzaldehyde	12	0	0	1	1
782	saturated hydrocarbon	1	0	0	0	0
787	2-ethylhexanal	3	0	0	1	0
792	n-propylbenzene	9	0	0	1	0
811	C_3H_7-benzene isomer	9	1	1	1	1
813	benzonitrile	7	0	0	0	0

(continued)

Table B7 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
829	C_3H_7-benzene isomer	9	0	0	1	0
831	saturated hydrocarbon	1	0	0	0	0
839	phenol	15	0	0	0	0
848	saturated hydrocarbon	1	1	1	1	1
851	C_3H_7-benzene isomer	9	0	0	0	0
875	benzofuran	5	0	0	0	0
877	saturated hydrocarbon	1	1	1	1	1
886	C_3H_7-benzene isomer	9	1	1	1	1
896	n-octanal	3	1	0	0	0
917	n-decane	1	0	0	0	0
925	saturated hydrocarbon	1	0	0	0	0
930	octamethylcyclotetrasiloxane	1	0	0	0	0
936	saturated hydrocarbon	1	0	0	1	0
948	C_3H_7-benzene isomer	9	0	0	0	0
955	octamethylcyclotetrasiloxane	1	0	0	1	0
983	2-ethyl-1-hexanol	2	0	0	1	1
998	saturated hydrocarbon	1	1	1	1	1
1018	acetophenone	5	1	1	1	1
1021	saturated hydrocarbon	1	1	0	0	0
1026	unsaturated hydrocarbon	1	1	0	0	0
1039	C_4H_9-benzene isomer	9	0	0	0	0
1065	saturated hydrocarbon	1	1	0	1	1
1078	saturated hydrocarbon	1	0	0	0	0
1079	unsaturated hydrocarbon	1	0	0	0	0
1083	cresol isomer	15	0	0	0	0
1088	saturated hydrocarbon	1	0	0	1	0
1098	C_4H_9-benzene isomer	9	0	0	0	0
1115	saturated hydrocarbon	1	0	0	0	0
1131	n-nonanal	3	1	1	1	1
1163	n-undecane	1	0	0	1	0
1175	C_4H_9-benzene isomer	9	0	0	0	0
1239	C_2H_5-phenol isomer	15	0	0	1	0
1287	naphthalene	9	1	1	1	1
1309	decamethylcyclopentasiloxane	1	0	0	0	0
1346	n-decanal	3	1	1	1	1
1374	saturated hydrocarbon	1	0	0	1	0
1507	methylnaphthalene isomer	9	0	0	1	0
1524	n,n-di-nor-butyl formamide	8	0	0	0	0
1564	saturated hydrocarbon	1	0	0	1	0
1632	alkyl butyrate compound	4	1	1	0	1
1640	silane compound	1	1	1	0	1
1665	alkyl butyrate compound	4	1	1	0	0
1738	saturated hydrocarbon	1	0	0	1	0
1839	unsaturated hydrocarbon	1	0	0	0	0
1894	saturated hydrocarbon	1	0	0	1	1

(continued)

Table B7 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
1922	silane compound	1	0	0	0	0
1978	diethyl o-phthalate	4	0	0	1	1
2027	2,2,4-trimethyl penta-1,3-diol di-isobutyrate	4	0	0	0	0
2040	benzophenone	5	1	1	0	0

Table B8. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 4 (LOCATION-1, VOL-L)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
62	trichlorofluoromethane	10	0	0	1	1
64	acetone	5	0	1	0	1
77	dichloromethane	10	1	1	0	1
106	2-methylpentane	1	0	1	1	0
134	hexafluorobenzene	11	1	1	1	1
136	n-hexane	1	0	1	1	1
143	chloroform	10	0	0	1	1
146	ethyl acetate	4	0	1	0	0
165	$C_6H_{14}O$ isomer	4	0	0	0	0
174	perfluorotoluene	11	1	1	1	1
178	1,1,1-trichloroethane	10	1	0	0	0
197	benzene	9	1	1	1	1
223	n-butyl alcohol	2	0	0	1	1
276	n-heptane	1	0	0	1	0
307	methylcyclohexane	1	0	1	1	1
375	toluene	9	1	1	1	1
478	saturated hydrocarbon	1	0	0	1	0
488	acetic acid	14	1	1	1	1
548	hexamethylcyclotrisiloxane	1	0	0	0	0
613	ethylbenzene	9	0	0	0	0
674	saturated hydrocarbon	1	0	0	1	0
676	unsaturated hydrocarbon	1	0	0	0	0
688	saturated hydrocarbon	1	0	0	1	0
718	saturated hydrocarbon	1	0	0	1	0
762	saturated hydrocarbon	1	0	0	1	0
794	benzaldehyde	12	0	0	1	1
837	benzonitrile	7	0	0	1	0
855	saturated hydrocarbon	1	0	0	1	0
874	saturated hydrocarbon	1	1	1	1	1
904	saturated hydrocarbon	1	1	1	1	1
912	C_3H_7-benzene isomer	9	0	0	0	0
913	saturated hydrocarbon	1	0	0	1	0
919	phenol	15	0	0	0	0
923	saturated hydrocarbon	1	0	0	1	0
943	saturated hydrocarbon	1	0	0	0	0
952	saturated hydrocarbon	1	0	0	1	0
956	octamethylcyclotetrasiloxane	1	0	0	0	0
965	saturated hydrocarbon	1	0	0	1	0
982	octamethylcyclotetrasiloxane	1	0	0	1	1
1009	2-ethyl-1-hexanol	2	0	0	1	0
1024	saturated hydrocarbon	1	1	1	1	0
1042	acetophenone	5	1	1	1	1
1086	saturated hydrocarbon	1	0	0	1	0
1109	cresol isomer	15	1	1	1	1
1143	N-nonanal	3	1	1	1	1

(continued)

Table B8 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
1175	saturated hydrocarbon	1	0	0	0	0
1244	dimethylphenol isomer	15	1	1	1	0
1247	dimethylphenol isomer	15	1	1	1	1
1290	C_2H_5-phenol isomer	15	1	1	1	1
1296	naphthalene	9	0	0	0	0
1302	C_2H_5-phenol isomer	15	1	1	1	1
1315	decamethylcyclopentasiloxane	1	0	0	0	0
1352	n-decanal	3	0	0	1	0
1421	unsaturated hydrocarbon	1	0	0	0	0
1454	saturated hydrocarbon	1	0	0	0	0
1512	methylnaphthalene isomer	9	0	0	0	0
1528	n,n-di-nor-butyl formamide	8	0	0	0	0
1540	saturated hydrocarbon	1	0	0	0	0
1636	alkyl butyrate compound	4	0	0	0	0
1643	silane compound	1	0	1	0	0
1665	alkyl butyrate compound	4	1	1	1	1
1739	saturated hydrocarbon	1	0	0	0	0
1879	saturated hydrocarbon	1	0	0	1	0
1902	silane compound	1	0	0	0	0
1959	diethyl o-phthalate	4	0	0	1	0
2003	2,2,4-trimethyl penta-1,3-diol di-isobutyrate	4	0	0	0	0
2021	benzophenone	5	0	0	0	0

Table B9. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 5 (LOCATION-1, VOL-L)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
84	acetone	6	0	0	0	0
88	trichlorofluoromethane	10	0	0	1	1
104	carbon disulfide	13	0	0	1	0
152	hexafluorobenzene	11	1	0	1	0
190	perfluorotoluene	11	1	0	1	0
211	benzene	9	0	1	1	1
266	trichloroethylene	10	1	1	1	1
387	toluene	9	1	1	1	1
485	saturated hydrocarbon	1	0	0	1	0
548	hexamethylcyclotrisiloxane	1	0	0	0	0
610	ethylbenzene	9	0	0	0	0
710	saturated hydrocarbon	1	0	0	0	0
774	benzaldehyde	12	0	0	1	0
854	saturated hydrocarbon	1	0	0	1	0
893	C_3H_7-benzene isomer	9	0	0	1	0
902	saturated hydrocarbon	1	0	0	1	0
964	octamethylcyclotetrasiloxane	1	0	0	1	1
991	2-ethyl-1-hexanol	2	0	0	1	0
1007	saturated hydrocarbon	1	0	0	1	0
1022	acetophenone	6	0	0	1	1
1026	saturated hydrocarbon	1	0	0	0	0
1061	cresol isomer	15	0	0	0	0
1076	cresol isomer	15	0	0	0	0
1128	n-nonanal	3	0	0	1	1
1229	dimethylphenol isomer	15	1	1	1	1
1273	dimethylphenol isomer	15	1	0	0	0
1282	naphthalene	9	0	0	0	0
1302	decamethylcyclopentasiloxane	1	0	0	0	0
1497	methylnaphthalene isomer	9	0	0	1	0
1626	silane compound	1	1	1	0	0
1649	butyl-n-butyrate isomer or other alkyl butyrate compound	4	1	1	1	1
1865	saturated hydrocarbon	1	0	0	0	0
1888	silane compound	1	0	0	0	0
1943	phthalate compound	4	1	1	1	1
1981	2,2,4-trimethylpenta-1,2-diol di-isobutyrate	4	0	0	0	0

Table B10. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 6 (LOCATION-1, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
45	acetone	6	0	0	0	0
51	trichlorofluoromethane	10	0	0	1	1
66	dichloromethane	10	1	1	0	1
70	carbon disulfide	13	0	0	0	0
94	C_6H_{14} isomer	1	0	0	0	0
109	acetic acid	14	0	0	0	0
119	hexafluorobenzene	11	1	1	1	1
122	n-hexane	1	0	0	0	0
127	chloroform	10	0	0	0	0
149	methylcyclopentane	1	0	1	1	1
157	perfluorotoluene	11	1	1	1	1
160	1,1,1-trichloroethane	10	0	1	0	0
179	benzene	9	1	1	1	1
185	carbon tetrachloride	10	0	0	0	0
189	cyclohexane	1	0	1	1	1
204	C_7H_{16} isomer	1	0	1	1	1
217	C_7H_{16} isomer	1	1	1	1	1
256	n-heptane	1	1	1	1	1
287	methylcyclohexane	1	0	1	1	1
355	toluene	9	1	1	1	1
375	acetic acid	14	0	0	1	0
383	C_8H_{18} isomer	1	1	1	1	1
398	C_8H_{18} isomer & C_8H_{16} isomer	1	1	1	0	1
413	saturated hydrocarbon	1	0	0	0	0
456	n-octane	1	1	1	1	1
503	unsaturated hydrocarbon(s)	1	0	0	1	0
516	unsaturated hydrocarbon	1	0	0	0	0
522	saturated hydrocarbon	1	0	0	0	0
527	C_9H_{18} isomer	1	0	0	1	0
533	C_9H_{18} isomer	1	0	1	1	0
555	C_9H_{18} isomer	1	0	0	1	0
560	ethylbenzene	9	0	1	1	1
569	C_9H_{18} isomer	1	0	0	0	0
581	xylene isomer	9	1	1	1	1
588	unsaturated hydrocarbon	1	0	0	0	0
606	saturated hydrocarbon	1	0	0	0	0
609	unsaturated hydrocarbon	1	0	0	1	0
623	styrene	9	1	1	1	1
633	o-xylene	9	1	1	1	1
655	saturated hydrocarbon	1	0	1	1	0
680	unsaturated hydrocarbon	1	0	0	0	0
690	saturated hydrocarbon	1	1	1	1	1
714	isopropylbenzene	9	0	0	0	0
730	saturated hydrocarbon	1	1	1	0	1
761	benzaldehyde	12	0	0	1	1

(continued)

Table B10 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
776	saturated hydrocarbon	1	0	0	0	0
785	n-propylbenzene	9	0	0	1	1
795	phenol	15	0	0	0	0
801	benzonitrile	7	0	0	0	0
805	C_3H_7 - benzene isomer	9	1	1	1	1
824	C_3H_7 - benzene isomer	9	1	1	1	1
843	saturated hydrocarbon	1	1	1	1	1
846	C_3H_7 - benzene isomer	9	1	0	0	0
872	saturated hydrocarbon	1	0	1	1	1
877	methylstyrene isomer	9	0	0	0	0
882	C_3H_7 - benzene isomer	9	1	1	1	1
892	n-octanal	3	1	1	0	1
905	dichlorobenzene isomer	11	0	0	0	0
912	saturated hydrocarbon	1	1	1	1	1
920	saturated hydrocarbon	1	0	0	0	0
927	octamethylcyclotetrasiloxane	1	0	0	0	0
932	saturated hydrocarbon	1	1	1	1	1
944	C_3H_7 - benzene isomer	9	0	1	1	1
951	octamethylcyclotetrasiloxane	1	0	0	1	1
968	indan or C_9H_{10} isomer	1	0	0	0	0
976	2-ethyl-1-hexanol	2	0	1	1	1
982	methylphenylacetylene	9	0	0	0	0
994	saturated hydrocarbon	1	1	1	1	1
1011	acetophenone	5	1	1	1	1
1015	saturated hydrocarbon	1	1	0	0	1
1026	C_4H_9 - benzene isomer	9	0	0	0	0
1033	C_4H_9 - benzene isomer	9	1	0	1	1
1049	C_4H_9 - benzene isomer	9	0	0	0	0
1061	cresol isomer	15	0	0	0	0
1071	C_4H_9 - benzene isomer	9	0	0	0	0
1076	cresol isomer	15	0	0	0	0
1078	$C_{10}H_{12}$ isomer (methylindan isomer or ethylstyrene isomer)	1	0	0	0	0
1082	C_4H_9 - benzene isomer	9	1	1	0	1
1109	n-nonanal	3	1	1	1	1
1135	saturated hydrocarbon	1	1	1	1	1
1140	C_4H_9 - benzene isomer	9	0	1	0	0
1147	C_4H_9 - benzene isomer	9	0	1	0	1
1175	$C_{10}H_{12}$ isomer (methylindan)	1	0	0	0	0
1200	dimethylphenol isomer	15	1	1	1	1
1243	dimethylphenol isomer	15	1	1	0	1
1250	naphthalene	9	0	0	1	1
1268	decamethylcyclopentasiloxane	1	0	0	0	0
1301	C_5H_{11} - benzene isomer	9	0	0	0	0
1306	n-decanal	3	1	1	1	1

(continued)

Table B10 (cont'd.)

Scan No.	Chemical	Class No.	HSSS		Incos	
			ND	D	ND	D
1320	C_5H_{11} - benzene isomer	9	0	0	0	0
1333	saturated hydrocarbon	1	1	1	1	1
1421	saturated hydrocarbon	1	0	0	0	0
1430	methylnaphthalene isomer	9	1	1	1	1
1437	3-methyl acetylacetone	5	0	0	0	0
1446	methylnaphthalene isomer	9	1	0	1	0
1457	saturated hydrocarbon	1	1	1	1	1
1516	silane compound	1	0	0	0	0
1548	biphenyl	9	0	0	0	0
1553	alkyl butyrate compound	4	1	1	1	0
1593	saturated hydrocarbon	1	0	0	0	0
1630	saturated hydrocarbon and C_2H_5 - alkyl naphthalene isomer	1	1	0	1	0
1725	saturated hydrocarbon	1	1	0	0	1
1765	saturated hydrocarbon	1	1	1	1	0
1861	diethyl o-phthalate	4	0	0	1	0

Table B11. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLES FROM SITE NO. 6 (LOCATION-2, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
61	trichlorofluoromethane	10	0	0	1	1
67	acetone	5	0	0	0	0
77	dichloromethane	10	0	1	0	1
80	carbon disulfide	13	0	1	0	0
105	C_6H_{14} isomer	1	0	1	1	1
116	3-methylpentane	1	0	1	1	1
132	hexafluorobenzene	11	1	1	1	1
133	n-hexane	1	0	0	0	0
140	chloroform	10	0	0	0	0
162	methylcyclopentane	1	0	0	1	1
171	perfluorotoluene	11	1	1	1	1
175	1,1,1-trichloroethane	10	1	1	0	0
195	benzene	9	0	1	1	1
204	cyclohexane	1	0	1	1	1
220	2-methylhexane	1	0	1	1	1
233	3-methylhexane	1	1	1	1	1
247	acetic acid	14	0	1	1	1
276	n-heptane	1	1	1	1	1
307	methylcyclohexane	1	1	1	1	1
337	C_8H_{18} isomer	1	0	0	1	0
376	toluene	9	1	1	1	1
403	C_8H_{18} isomer	1	1	1	1	0
418	C_8H_{18} and C_8H_{16} isomers	1	0	1	1	1
447	unsaturated hydrocarbon	1	0	0	0	0
476	saturated hydrocarbon	1	1	1	1	1
500	acetic acid	14	0	0	1	0
541	unsaturated hydrocarbon	1	0	0	0	0
563	saturated hydrocarbon	1	0	0	0	0
587	ethylbenzene	9	1	1	1	1
610	xylene isomer	9	1	1	1	1
635	saturated hydrocarbon	1	0	0	1	0
653	saturated hydrocarbon	1	0	0	0	0
654	styrene	9	0	0	0	0
664	xylene isomer	9	1	1	0	1
675	unsaturated hydrocarbon	1	0	0	0	0
720	saturated hydrocarbon	1	1	1	1	1
792	benzaldehyde	12	0	0	1	1
806	saturated hydrocarbon	1	0	0	1	0
816	n-propylbenzene	9	0	0	0	0
836	C_3H_7 - benzene isomer	9	0	0	1	0
854	C_3H_7 - benzene isomer	9	1	1	0	1
873	saturated hydrocarbon	1	1	1	1	1
876	C_3H_7 - benzene isomer	9	0	0	0	0
895	saturated hydrocarbon	1	0	0	1	0

(continued)

Table B11 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
906	phenol	15	0	0	0	0
908	methylstyrene isomer	9	0	0	0	0
912	C_3H_7 - benzene isomer	9	1	1	1	1
922	n-octanal	3	1	0	0	0
935	dichlorobenzene isomer	11	0	0	1	0
963	saturated hydrocarbon	1	0	0	0	1
974	C_3H_7 - benzene isomer	9	0	0	0	0
981	octamethylcyclotetrasiloxane	1	0	0	1	0
995	methylstyrene isomer	9	0	0	0	0
1002	2-ethyl-1-hexanol	2	0	0	0	0
1004	methylphenylacetylene C_9H_8	9	0	0	0	0
1007	saturated hydrocarbon	1	0	0	0	0
1012	saturated hydrocarbon	1	0	0	1	0
1026	acetophenone	5	1	1	1	1
1031	C_4H_9 - benzene isomer	9	0	0	1	0
1044	C_4H_9 - benzene isomer	9	0	0	1	0
1079	saturated hydrocarbon	1	0	0	0	0
1085	C_4H_9 - benzene isomer	1	0	0	0	0
1093	cresol isomer	15	0	0	1	0
1098	C_4H_9 - benzene isomer	9	0	0	1	0
1129	n-nonanal	3	1	1	1	1
1163	saturated hydrocarbon	1	1	0	1	1
1168	C_4H_9 - benzene isomer	9	0	0	1	0
1175	C_4H_9 - benzene isomer	9	0	0	1	0
1238	dimethylphenol isomer	15	1	0	1	1
1282	C_2H_5 - phenol isomer	15	1	0	1	0
1288	naphthalene	9	0	0	1	1
1295	C_2H_5 - phenol isomer	15	0	0	1	0
1307	decamethylcyclopentasiloxane	1	0	0	0	1
1346	n-decanal	3	0	0	1	0
1374	saturated hydrocarbon	1	1	0	1	1
1406	saturated hydrocarbon	1	0	0	0	0
1466	saturated hydrocarbon	1	0	0	1	0
1477	methylnaphthalene isomer	9	1	1	1	1
1499	methylnaphthalene isomer	9	0	0	0	0
1517	saturated hydrocarbon	1	1	0	1	1
1599	silane compound	1	0	0	0	0
1623	biphenyl	9	0	0	0	0
1628	alkyl butyrate compound	4	0	0	1	0
1661	diphenyl ether	5	0	0	0	0
1668	saturated hydrocarbon	1	0	0	0	0
1676	C_2H_5 - naphthalene isomer	9	0	0	0	0
1702	C_2H_5 - naphthalene isomer	9	0	0	0	0
1707	saturated hydrocarbon	1	0	0	1	0
1805	saturated hydrocarbon	1	0	0	0	0
1867	saturated hydrocarbon		0	0	0	0
1971	diethyl o-phthalate	4	0	0	0	0

Table B12. CHEMICALS IDENTIFIED IN AMBIENT AIR SAMPLE FROM SITE NO. 7 (LOCATION-2, VOL-H)

Scan No.	Chemical	Class No.	MSSS		Incos	
			ND	D	ND	D
42	C_5H_{12} isomer(s)	1	0	1	0	0
49	trichlorofluoromethane	10	0	0	0	0
56	n-pentane	1	1	1	0	0
90	C_5H_{10} isomer	1	0	0	0	0
97	C_6H_{14} isomer	1	1	1	0	0
108	C_6H_{14} isomer	1	1	1	0	0
118	hexafluorobenzene	11	0	1	0	0
125	n-hexane	1	1	1	0	0
153	methylcyclopentane	1	0	1	0	0
159	perfluorotoluene	11	1	1	0	0
164	1,1,1-trichloroethane	10	0	0	0	0
183	benzene	9	1	1	0	0
194	cyclohexane	1	1	1	0	0
210	C_7H_{16} isomer	1	1	1	0	0
223	C_7H_{16} isomer	1	1	1	0	0
232	n-heptanol	2	0	0	0	0
266	$C_6H_{12}O$ isomer	2	0	0	0	0
296	methylcyclohexane	1	0	1	1	1
300	acetic acid	14	0	0	0	0
317	C_8H_{18} isomer	1	0	0	1	1
366	toluene	9	1	1	1	1
392	C_8H_{18} isomer	1	1	1	1	1
406	C_8H_{18} isomer	1	1	1	1	1
464	C_8H_{18} isomer	1	1	1	1	1
504	saturated hydrocarbon	1	0	0	0	0
511	saturated hydrocarbon	1	0	0	0	0
528	saturated hydrocarbon	1	0	0	1	1
543	saturated hydrocarbon	1	0	0	1	1
566	ethylbenzene	9	1	0	1	1
588	xylene isomer	9	1	1	1	1
609	saturated hydrocarbon	1	0	0	1	1
626	saturated hydrocarbon	1	0	0	1	1
628	styrene	9	0	0	0	0
637	xylene isomer	9	1	1	1	1
654	$C_7H_{14}O_2$ isomer	14	1	1	1	1
675	butyl proprionate isomer	4	0	0	1	1
682	saturated hydrocarbon	1	1	1	1	1
686	saturated hydrocarbon	1	1	1	1	1
694	$C_7H_{14}O_2$ isomer	4	0	0	1	1
724	saturated hydrocarbon	1	1	1	1	1
742	saturated hydrocarbon	1	0	0	1	1
755	benzaldehyde	12	1	0	1	1
768	saturated hydrocarbon	1	0	0	1	1
782	alkyl butyrate	4	1	1	1	1
783	saturated hydrocarbon	1	0	0	0	0

(continued)

Table B12 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			MD	D	MD	D
787	alkyl butyrate	4	1	1	1	1
798	C_3H_7 - benzene isomer	9	0	0	1	1
816	C_3H_7 - benzene isomer	9	0	0	1	1
836	saturated hydrocarbon	1	1	1	1	1
843	butyl crotonate or $C_8H_{14}O_2$ isomer	4	0	1	1	1
860	phenol	15	0	0	0	0
866	saturated hydrocarbon	1	1	1	1	1
876	C_3H_7 - benzene isomer	9	1	1	1	1
833	alkyl butyrate	4	1	1	0	0
887	saturated hydrocarbon	1	1	0	0	0
910	saturated hydrocarbon	1	1	1	1	1
928	saturated hydrocarbon	1	0	0	1	1
940	C_3H_7 - benzene isomer	9	0	0	0	0
945	unsaturated hydrocarbon	1	1	1	1	1
948	octamethylcyclotetrasiloxane	1	0	0	1	1
961	saturated hydrocarbon	1	0	0	0	0
973	2 - ethyl-1-hexanol	2	1	0	1	1
982	saturated hydrocarbon	1	1	1	0	0
989	saturated & unsaturated hydrocarbons	1	1	1	1	1
1005	acetophenone	5	1	1	1	1
1008	saturated hydrocarbon	1	1	1	1	1
1062	cresol isomer	15	1	0	1	1
1068	cresol isomer	15	1	0	1	1
1075	C_4H_5 - benzene isomer	9	0	0	1	1
1100	n-nonanal	3	1	1	1	1
1127	saturated hydrocarbon	1	1	1	1	1
1141	saturated hydrocarbon	1	1	0	1	1
1197	dimethylphenol isomer	15	1	1	1	1
1241	ethylphenol isomer	15	0	0	1	1
1253	naphthalene	9	0	0	1	1
1272	decamethylcyclopentasiloxane	1	0	0	0	0
1312	n-decanal	3	1	0	1	1
1338	saturated hydrocarbon	1	1	1	1	1
1371	saturated hydrocarbon	1	0	0	1	1
1407	unsaturated hydrocarbon	1	0	0	0	0
1432	saturated hydrocarbon	1	0	0	1	1
1444	saturated hydrocarbon	1	0	0	1	1
1451	saturated hydrocarbon	1	0	0	0	0
1464	methylnaphthalene isomer	9	0	0	0	1
1470	saturated hydrocarbon	1	1	0	1	1
1490	methylnaphthalene isomer	9	0	0	1	1
1493	unsaturated hydrocarbon	1	0	0	1	1
1518	saturated hydrocarbon	1	1	1	1	1
1557	saturated hydrocarbon	1	0	0	0	0
1605	silane compound	1	0	0	0	0

(continued)

Table B12 (cont'd.)

Scan No.	Chemical	Class No.	MSSS		Incos	
			MD	D	MD	D
1630	alkyl butyrate compound	4	0	1	0	0
1646	saturated hydrocarbon	1	0	0	0	0
1657	saturated hydrocarbon	1	0	0	0	0
1673	saturated hydrocarbon	1	0	0	0	0
1682	dimethylnaphthalene isomer	9	0	0	0	0
1695	unsaturated hydrocarbon	1	0	0	0	0
1705	dimethylnaphthalene isomer	9	0	0	0	0
1712	saturated hydrocarbon	1	1	1	0	0
1828	saturated hydrocarbon	1	0	0	0	0